INMOST – a software platform for distributed mathematical modelling

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ECCM-ECFD18

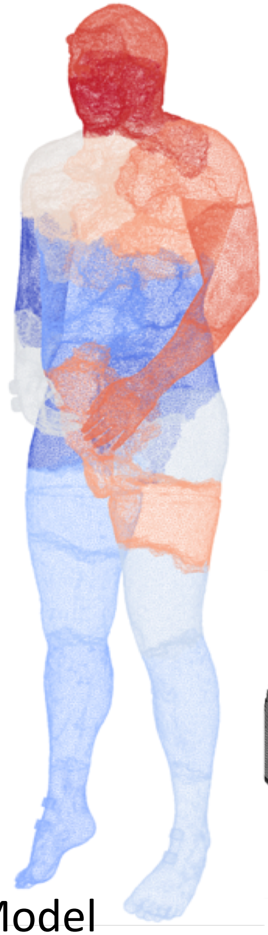
INMOST

functionality

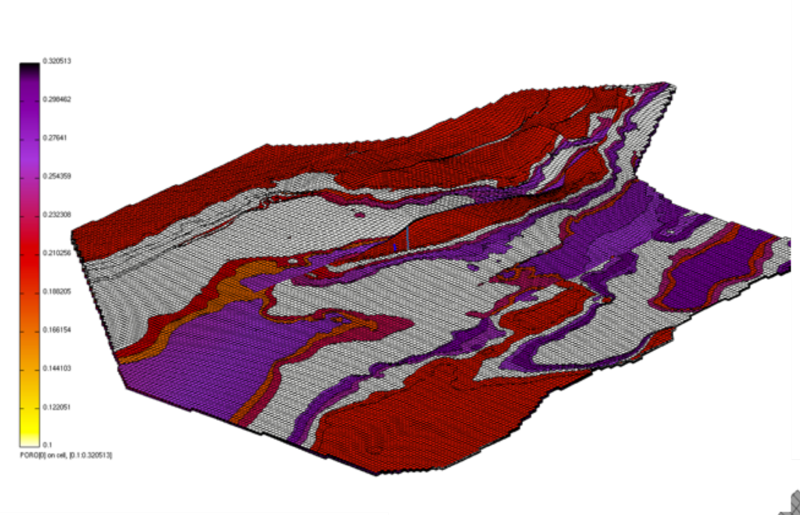
What is INMOST?

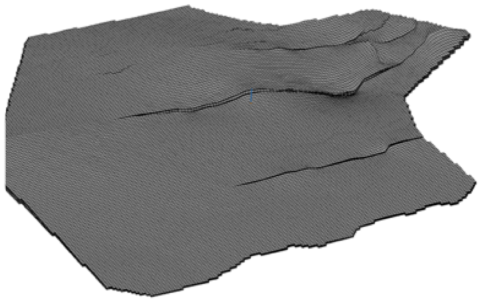
- **INMOST** abbreviation for (courtesy of Yuri):
  - Integrated
  - Numerical
  - **Modelling** and
  - Object-oriented
  - Supercomputing
  - Technologies
- Conceived during my internship at University of Houston / Exxon-Mobil in 2012.

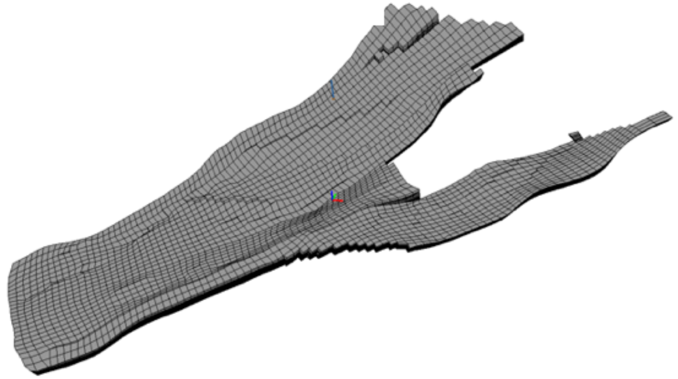
INMOST: Grids



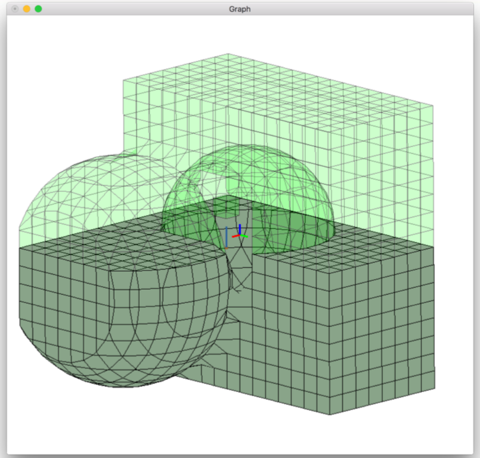
Model
Of human body



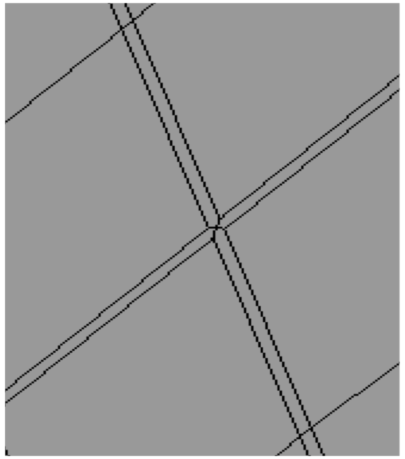




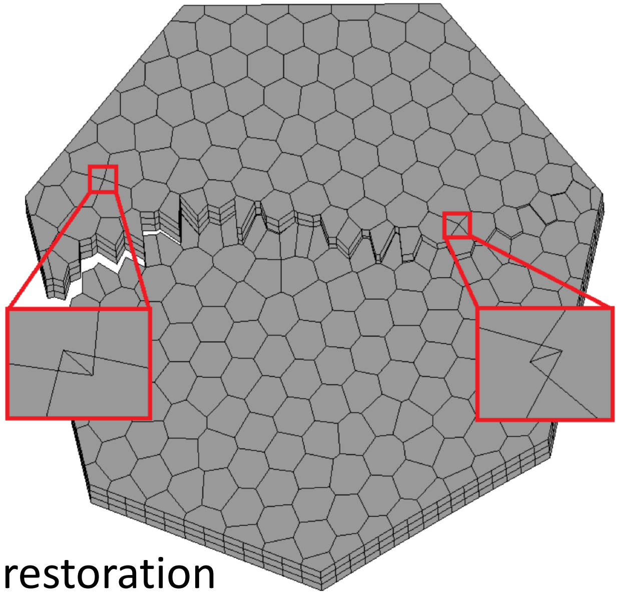
Geological grids with pinch-outs,
Supports Eclipse simulator format



Complex modifications

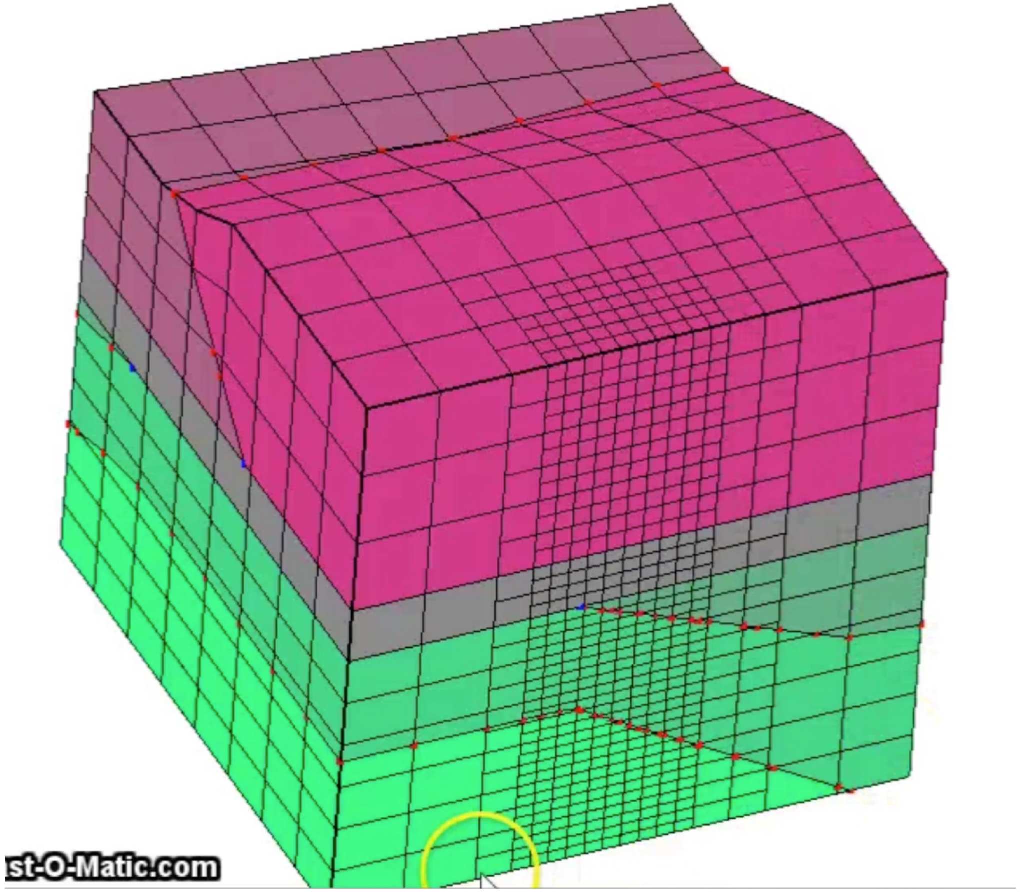


Cracking the mesh



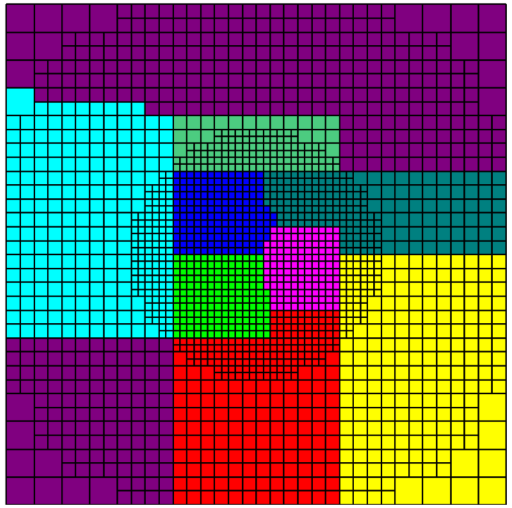
Grid restoration

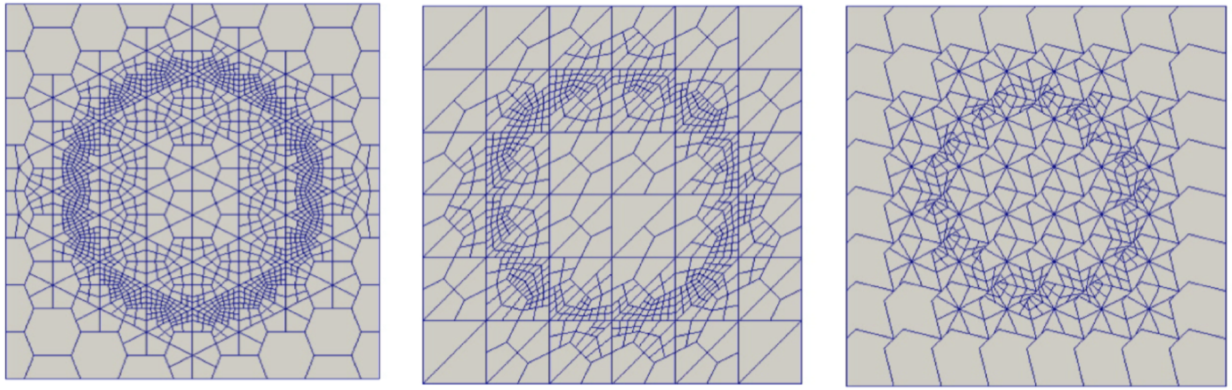
INMOST: Dynamic grids



Built-in OctreeCutcell example

Parallel scalable dynamic mesh
Adaptation and balancing

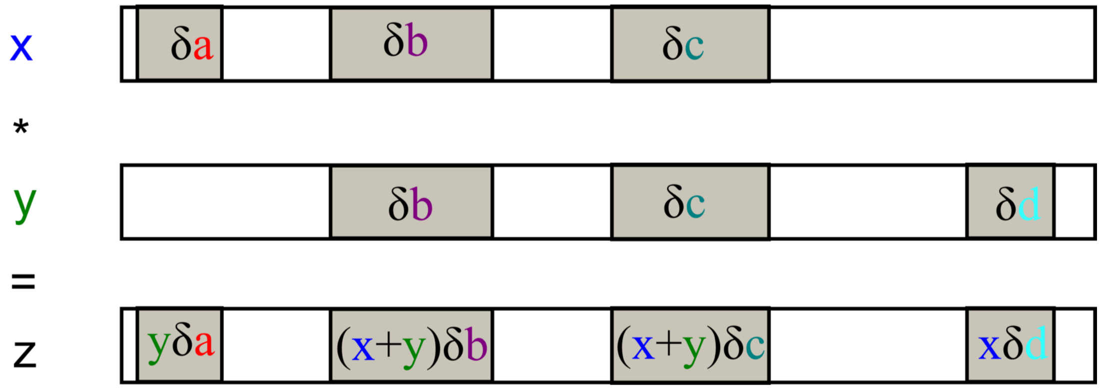




AdaptiveMesh example for general grid adaptation.

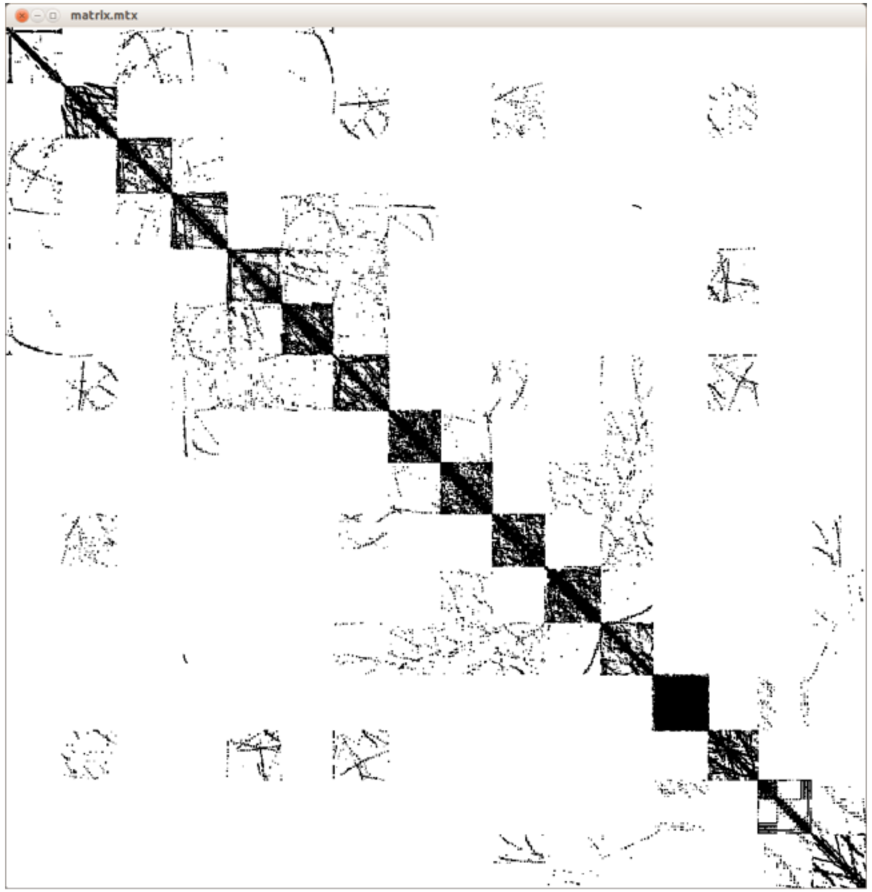
INMOST: Auto-differentiation

- Computes **Jacobian** matrix.
- Very **useful** for **complex** nonlinear problems.
- INMOST provides **BLAS-like** linear algebra functionality with automatic differentiation.
- Most modelling examples further use this functionality.



INMOST: Solvers

- **Easy** structures for assembly of distributed linear systems in parallel.
- **Distributed** solve:
  - Call to PETSc, Trilinos, SuperLU, Hypre.
  - Methods by Kaporin and Konshin.
  - My own developements.
- **Also**: mesh balancing and migration, any number of ghost layers, grid data exchange.



INMOST: Multiphysics

- Decouple simulator by **models**.
- Models are coupled by **functions**:
  - mobility, density, porosity, etc.
- Or by **coupling** terms:
  - Biot term, incompressibility, capillarity, etc.
- INMOST can **manage**:
  - Models, unknowns, functions, couplings, assembly of residual and Jacobian.
- **Fully implicit** solution.

Equations ↓ / Unknowns →	u,v,w	p	S_o, S_w, S_g	T
Elasticity	Deformation	Biot term	Capillary effects	Thermal expansion
Darcy	Biot term, rock porosity	Flow	Capillary effects	Thermal effects
Advection	Structure movement	Flow velocity, mobility	Fluids	Heat gradient
Conduction	Structure movement	Flow velocity	Density gradient	Thermal

Models and some couplings in **reservoir simulator**

INMOST: Users and development

- Users:
  - **INM RAS**;
  - **IBRAE RAS**, Rosatom – Ivan Kapyrin's lab, GeRa code;
  - **Stanford**, USA – group of Hamdi Tchelepi, AD-GPRS code;
  - Hariot-Watt, UK – Christina Mayer;
  - KHU, Qatar – Ahmad Abushaikha;
  - TU Delft, Holland – Denis Voskov.
- Occasionally:
  - Total, Chevron, Exxon-Mobil, Storengy, INPEX, Samsung, maybe Siemens.

- Further developments:
  - Multiphysics.
  - Linear solvers.
  - Detailed documentations.
  - FV-book with Springer.

В учебном пособии представлен опыт создания параллельной программной MPI-платформы и графической среды для разработки параллельных численных моделей на сетках общего вида. Технологический комплекс INMOST (Integrated Numerical Modeling and Object-oriented Supercomputing Technologies) – инструментарий для суперкомпьютерного моделирования, характеризуемый максимальной общностью поддерживаемых расчетных сеток, гибкостью и экономичностью структуры распределенных данных, кроссплатформенностью, а также графической средой для интерактивного пользовательского интерфейса.

Данное учебное пособие будет полезно разработчикам СИА, инженерам и математикам-вычислителям, деятельность которых связана с суперкомпьютерным моделированием: всем тем, кто непосредственно создает параллельные приложения или использует параллельные численные модели.

INMOST ПРОГРАММНАЯ ПЛАТФОРМА И ГРАФИЧЕСКАЯ СРЕДА

Серия Суперкомпьютерное Образование

Ю. В. Василевский, И. Н. Коньшин,
Г. В. Копытов, К. М. Терехов

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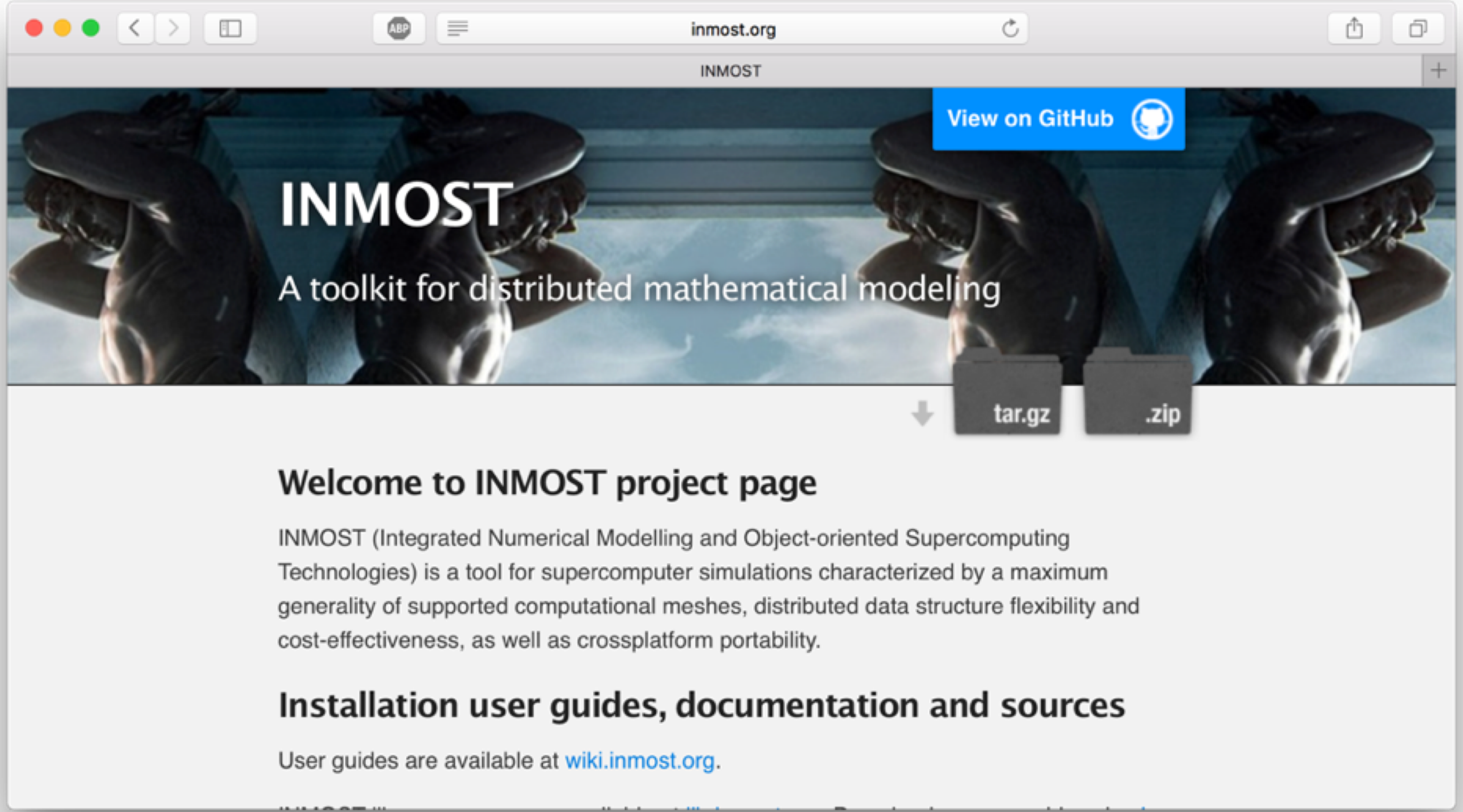

inmost.org
INMOST
View on GitHub
INMOST
A toolkit for distributed mathematical modeling
tar.gz
.zip
Welcome to INMOST project page
INMOST (Integrated Numerical Modelling and Object-oriented Supercomputing Technologies) is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility and cost-effectiveness, as well as crossplatform portability.
Installation user guides, documentation and sources
User guides are available at wiki.inmost.org.

INMOST: Today

- Supported open-source **BSD**-licensed project
- Exists on git on **http://github.com/INMOST-DEV/INMOST**
- Short address **http://www.inmost.org**
- Doxygen documentation: **http://doxy.inmost.org**
- Wiki documentation: **http://wiki.inmost.org**
- Many integrated examples and instruments.

Models

on INMOST

Models: Black-oil

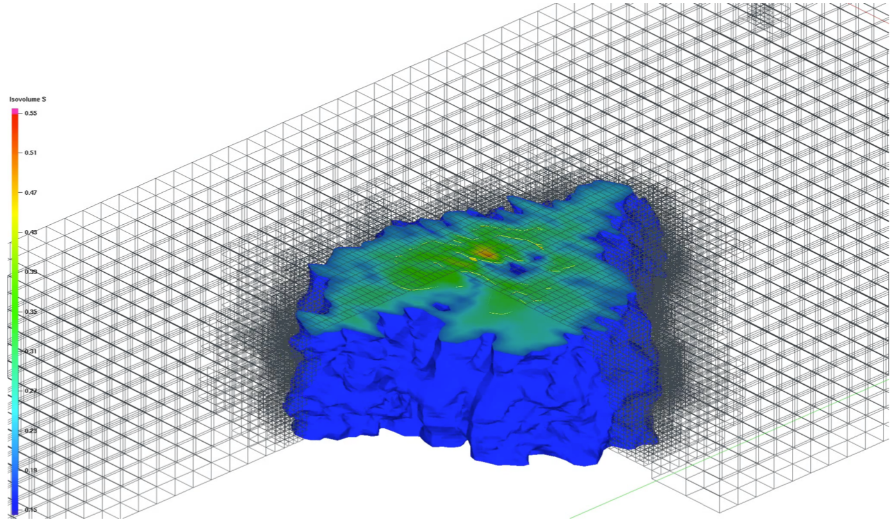
Unknowns: p, S_o, S_g or p_b depending on state

Equations:

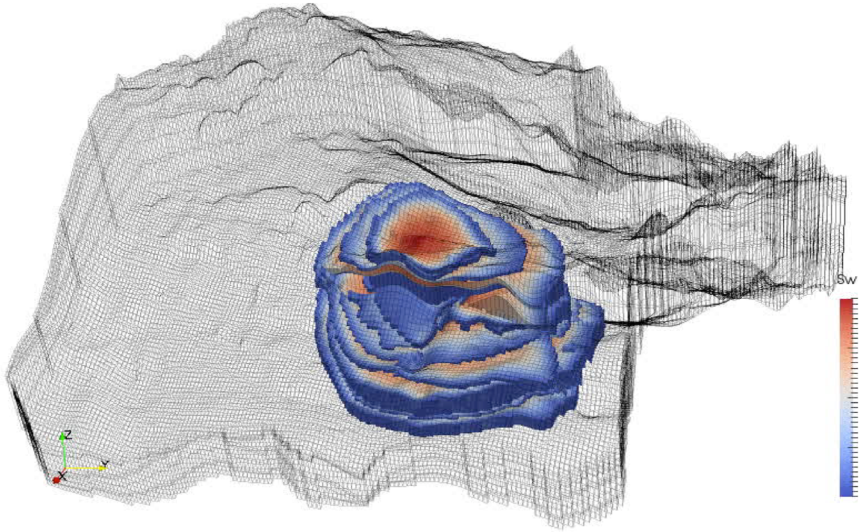
$$\frac{\partial \rho_w \theta S_w}{\partial t} - \nabla \cdot \left(\lambda_w \mathbb{K}(\nabla p - \rho_w g \nabla z)\right) = q_w$$

$$\frac{\partial \rho_o \theta S_o}{\partial t} - \nabla \cdot \left(\lambda_o \mathbb{K}(\nabla p - \nabla Pc_o - \rho_w g \nabla z)\right) = q_o$$

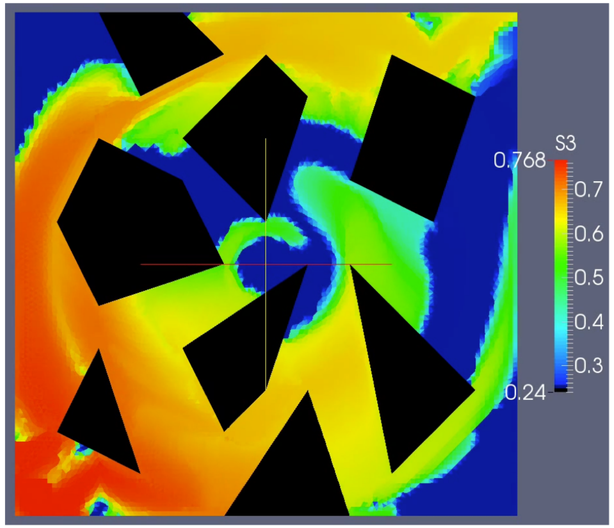
$$\frac{\partial \rho_g \theta \left(RS_o + S_g\right)}{\partial t} - \nabla \cdot \left(\lambda_g \mathbb{K}(\nabla p - \nabla Pc_g - \rho_g g \nabla z)\right) = q_g$$



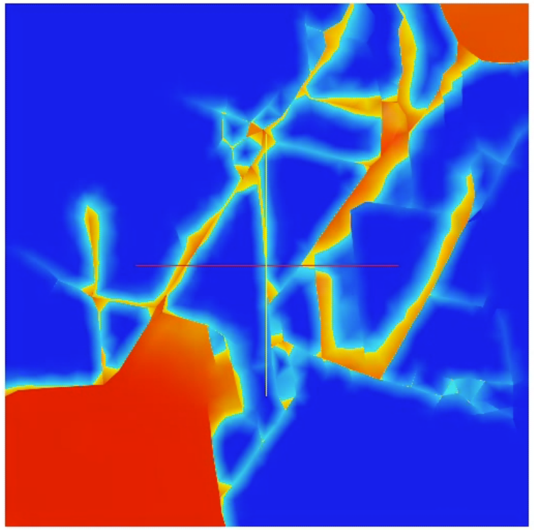
Dynamic grids, SPE10 based geology



Complex realistic geometry



Extreme anisotropy



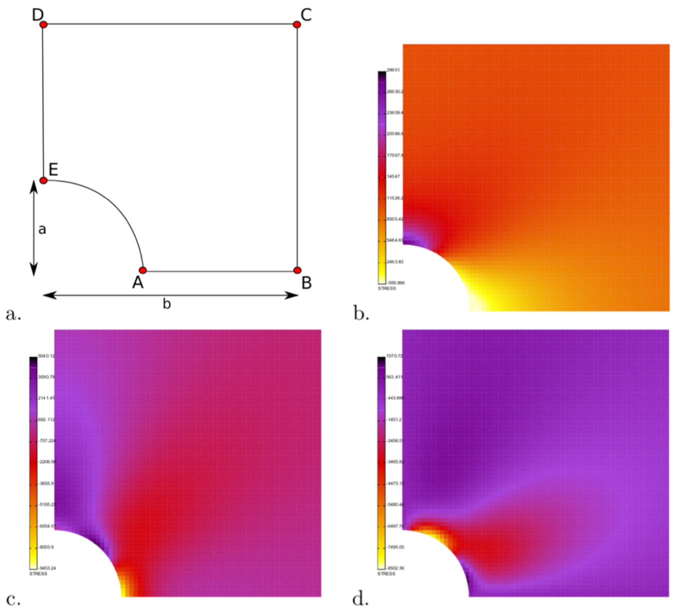
Fractures

Models: Linear elasticity

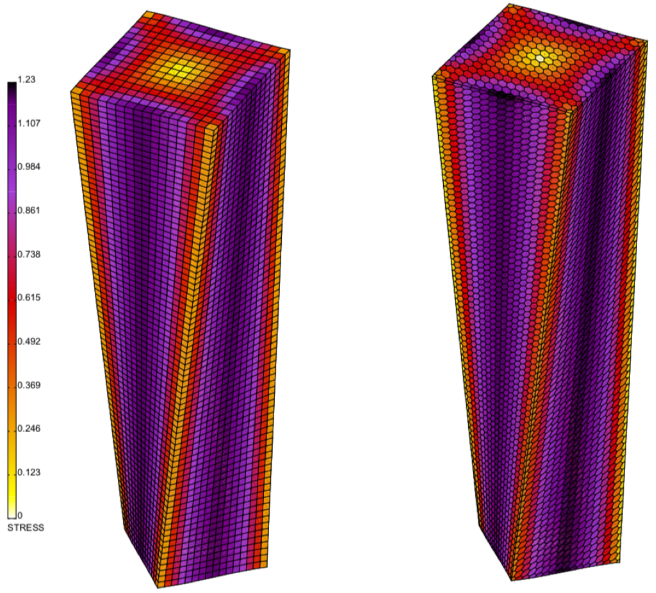
Unknowns: u, v, w

Equations:

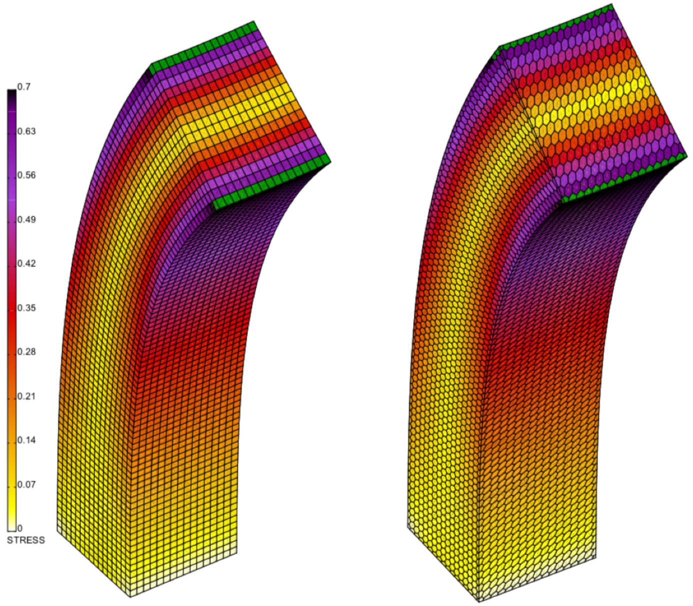
$$-\mathrm{div}(\boldsymbol{\sigma}) = 0,$$
$$\mathbb{C}:\boldsymbol{\sigma} = \frac{\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T}{2}$$



Loading



Twist



Bend

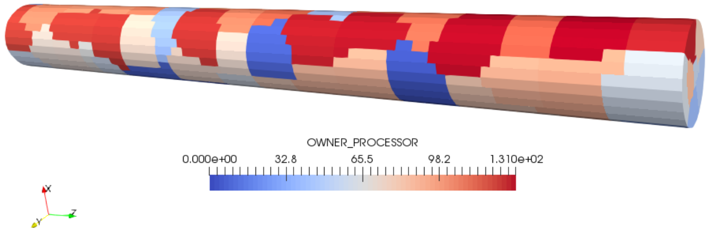
Models: Incompressible fluid

Unknowns: u, v, w, p

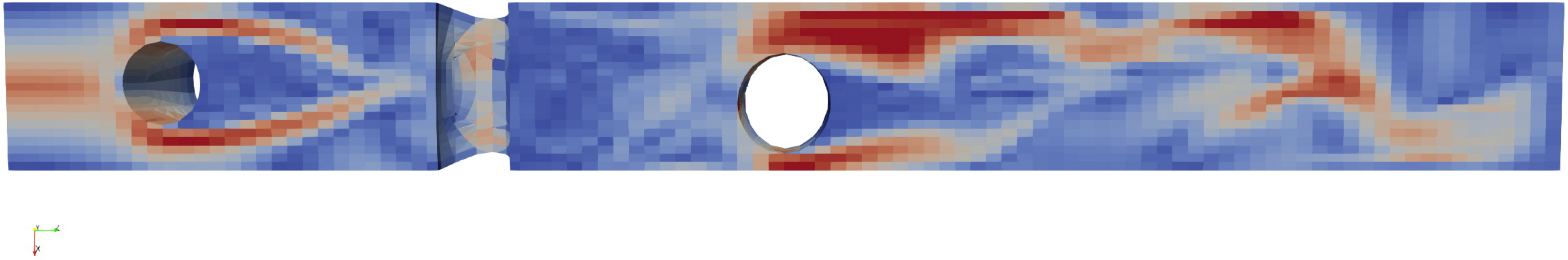
Equations:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \operatorname{div}\left(\rho \boldsymbol{u}\boldsymbol{u}^{\boldsymbol{T}} - \mu \nabla \boldsymbol{u} + pI\right) = 0$$

$$\operatorname{div}(\boldsymbol{u}) = 0$$



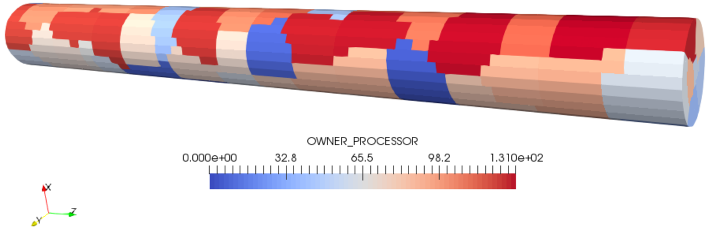
Parallel, one newton iteration:
36 procs: 2.51 sec
92 procs: 1.25 sec



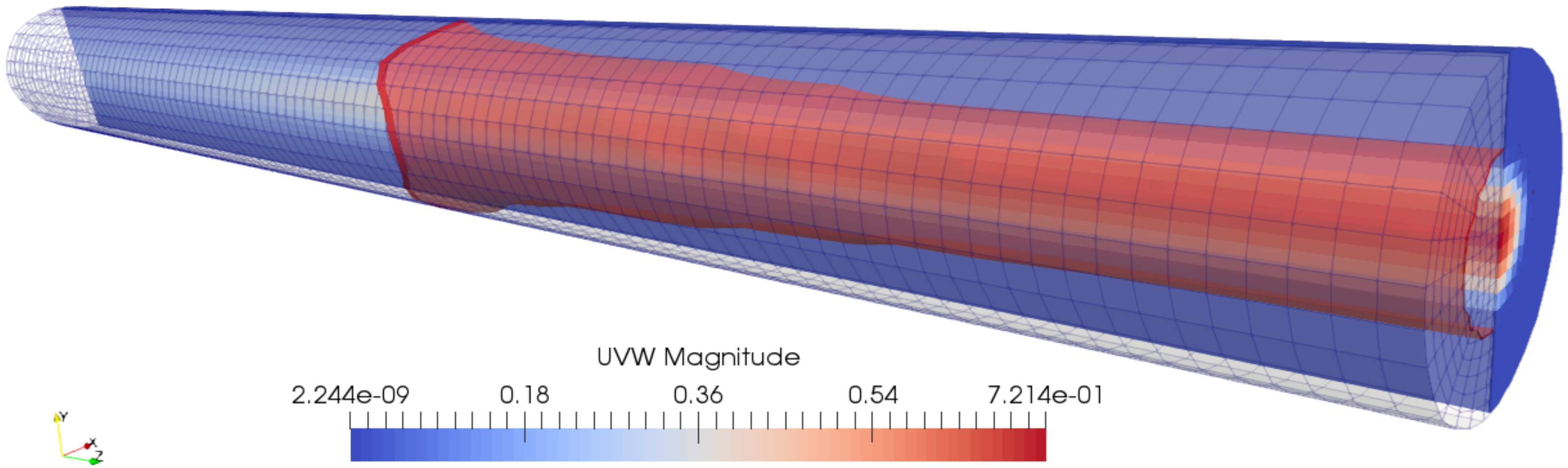
Models: Blood coagulation

Unknowns: $u, v, w, p, PT, T, A, Ba, F, Fp, Fg, \varphi_f, \varphi_c$

Equations: Incompressible N-S + Darcy, nonlinear advection-diffusion + reactions



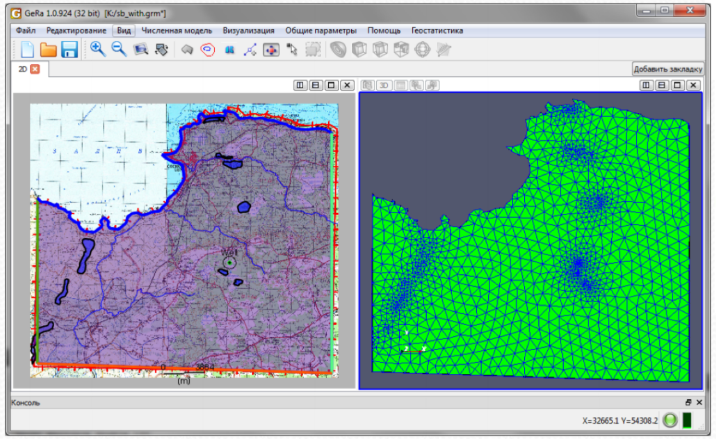
Using ~80 processors to simulate on fine mesh



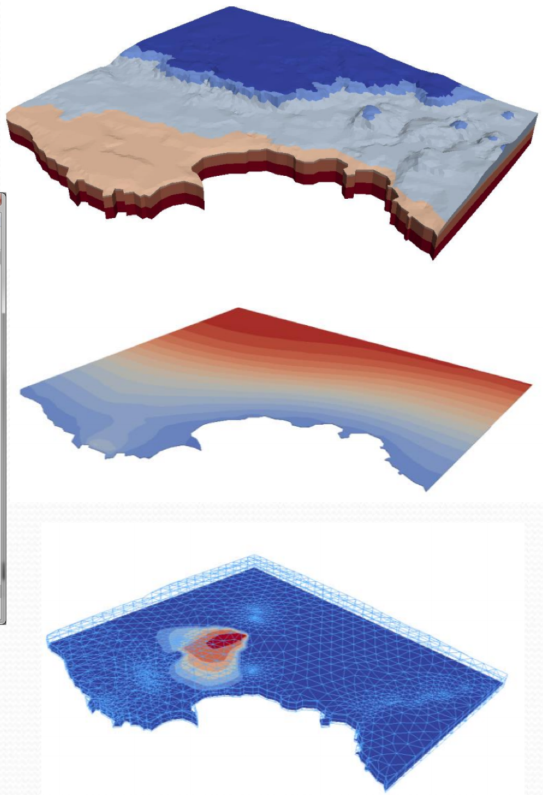
Models: Nuclear Waste Disposal (GeRa)

Mature end-user application with interface. Uses INMOST for mesh generation and parallel mesh management, solution of linear systems.

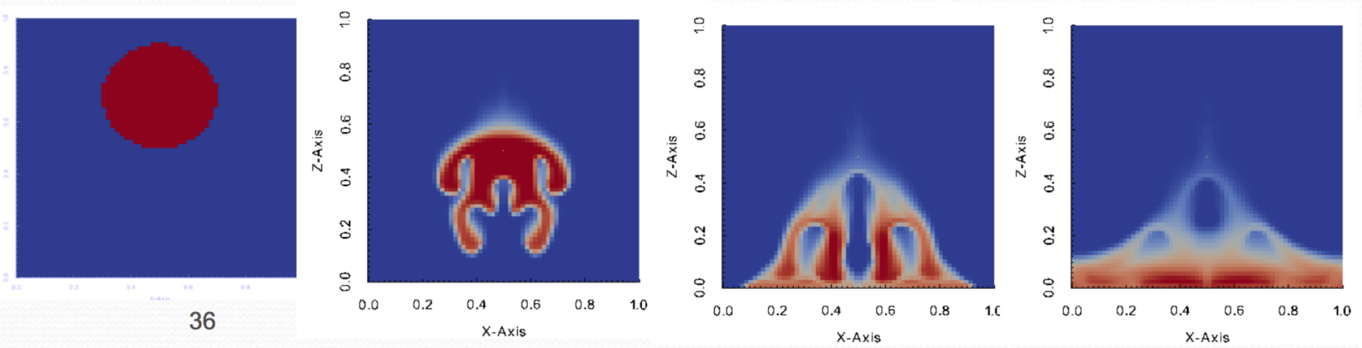
Physics:
- multiphase filtration;
- density convection;
- sorption;
- chemistry;
- …



Program interface



Simulation result

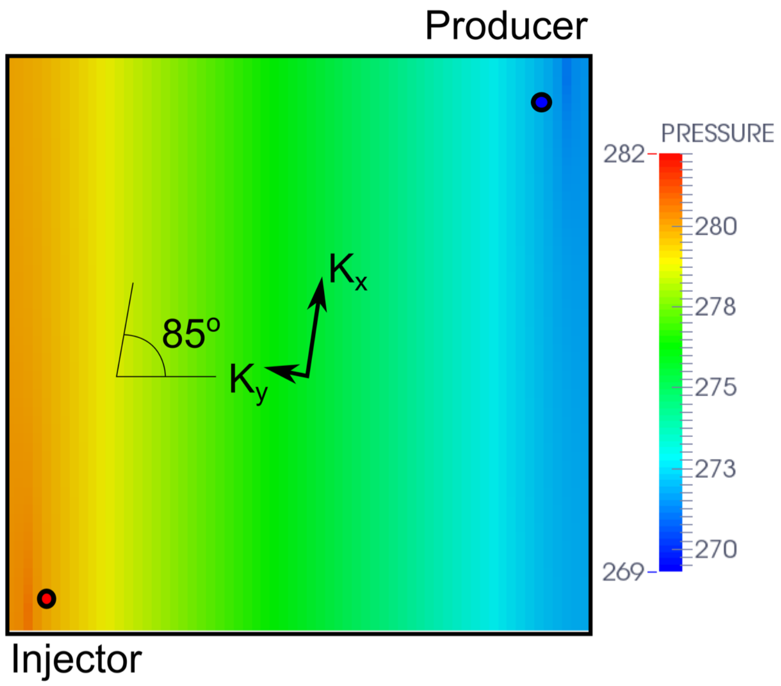


Density convection

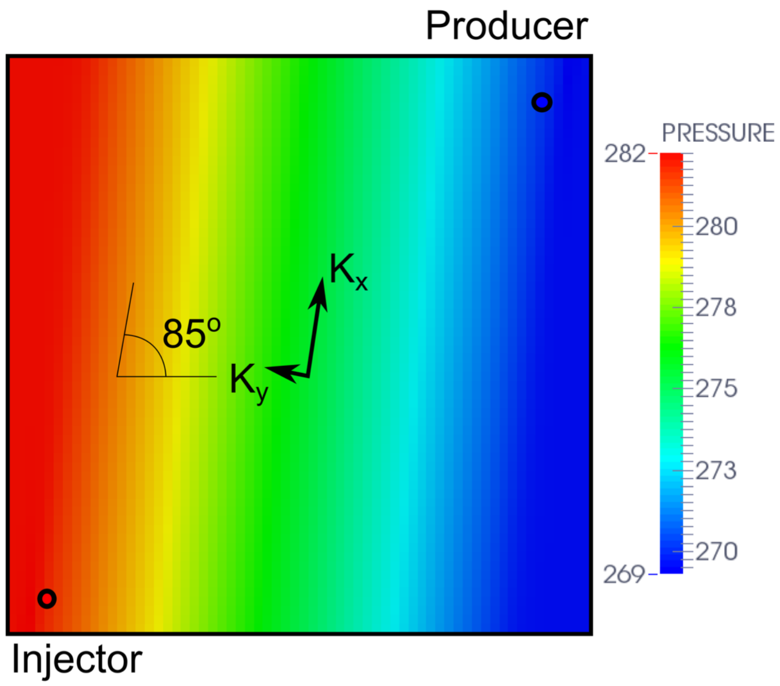
Finite-volume methods

for Multi-physics

Simple single phase diffusion problem

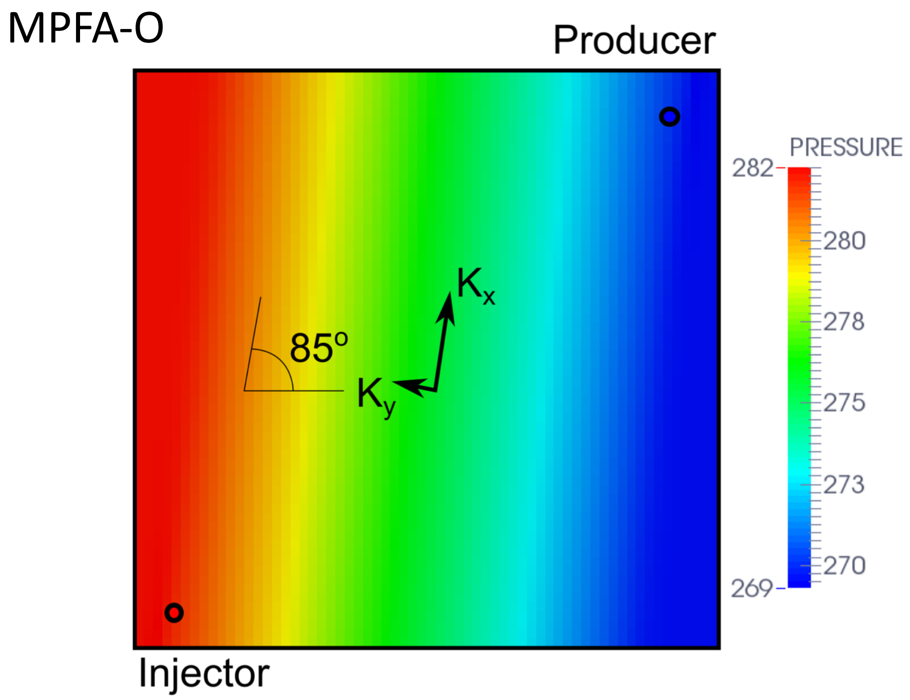


TPFA, O(1)-error, incorrect

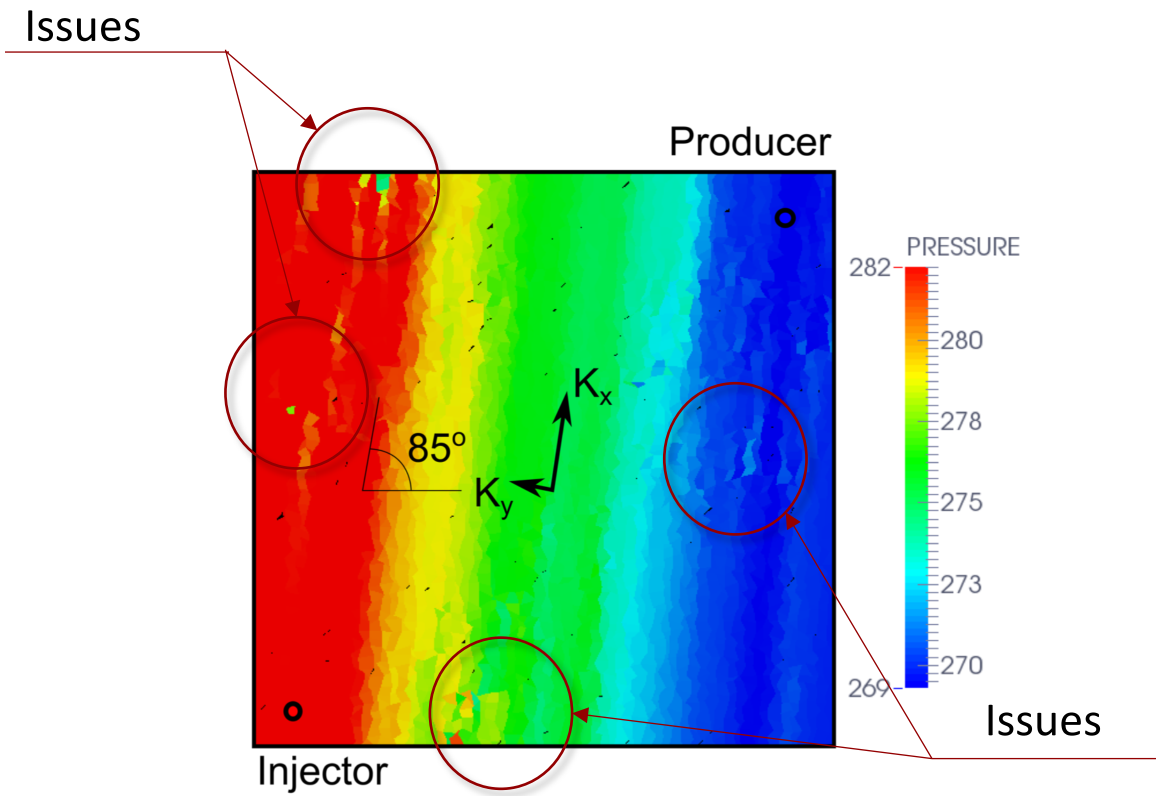


MPFA-O, O(h^2)-error, accurate

Simple single phase diffusion problem

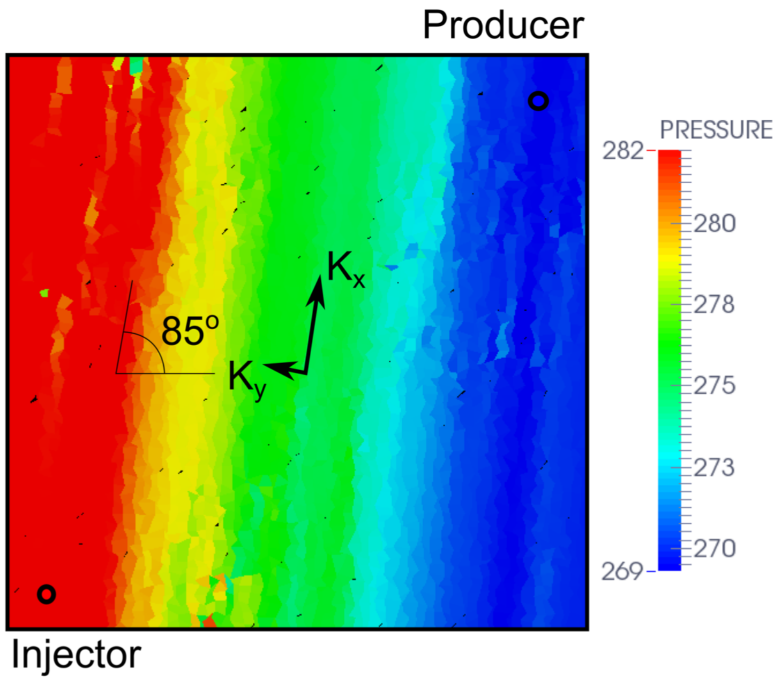


MPFA-O, Cartesian grid, accurate

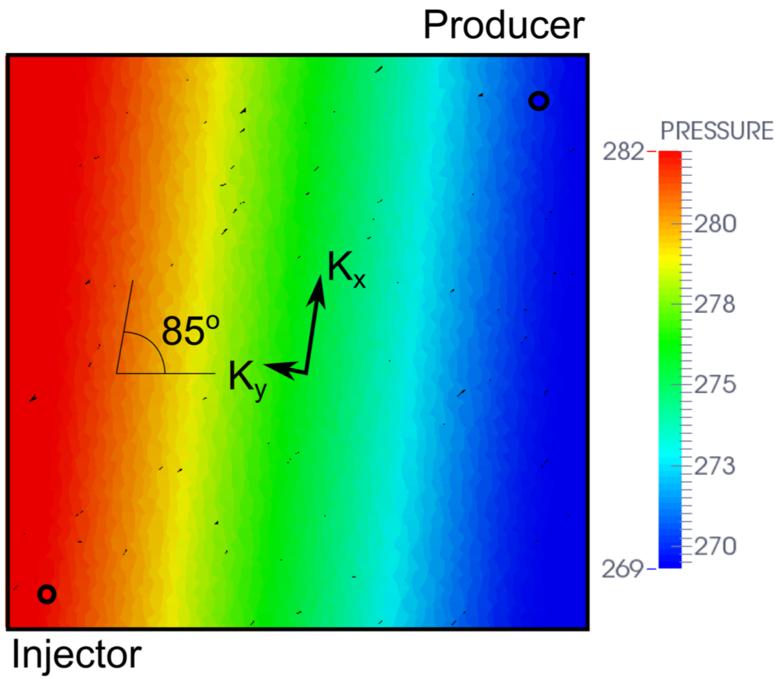


MPFA-O, skewed Cartesian grid, unstable

Simple single phase diffusion problem



MPFA-O, skewed Cartesian grid, unstable



Nonlinear scheme, skewed Cartesian grid, accurate

Transition to nonlinearity

No linear small stencil conservative scheme can be exact on linear solutions and respect the maximum principle.

[Kershaw 1981, Nordbotton 2005]

Diffusion Problem

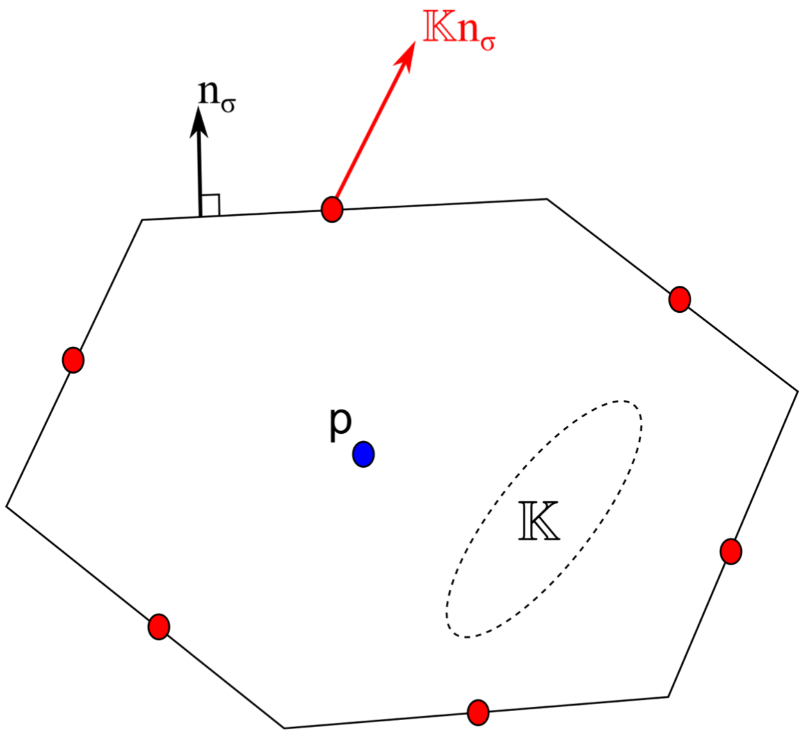
- The finite volume method uses Gauss law:

$$\int -\nabla \cdot \mathbb{K}\nabla p \, dV = \oint -\mathbb{K}\nabla p \cdot \boldsymbol{n}_f \, dS$$

- The scalar product in red has the alternative form:

$$\mathbb{K}\nabla p \cdot \boldsymbol{n}_f = \nabla p \cdot \mathbb{K}\boldsymbol{n}_f$$

- We express the flux along the direction of $\mathbb{K}\boldsymbol{n}_f$.



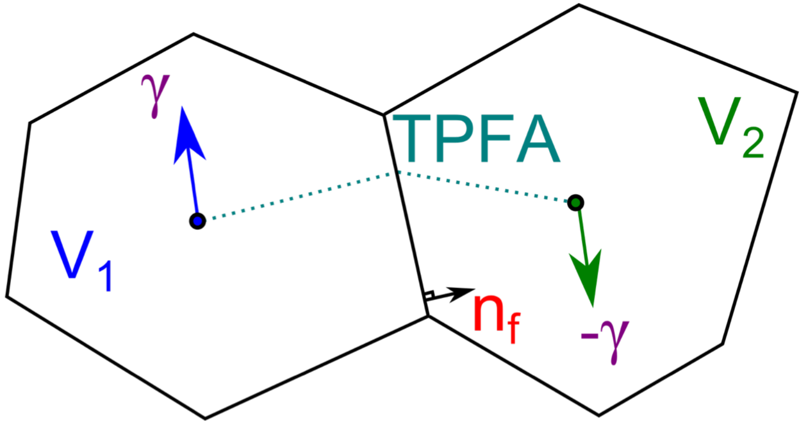
Diffusion Problem

- We need a gradient along vector:
  - $q = -(\mathbb{K}_1 \boldsymbol{n}_f) \cdot \nabla p = -(\mathbb{K}_2 \boldsymbol{n}_f) \cdot \nabla p$
- Two-point flux:

$$q_n = \frac{\lambda_1 \lambda_2}{\lambda_1 d_2 + \lambda_2 d_1}(p_2 - p_1)$$

- Lost transversal part of the flux:

$$q_\tau = \boldsymbol{\gamma} \cdot \nabla p = \frac{\lambda_1 \lambda_2 (\boldsymbol{y}_1 - \boldsymbol{y}_2) + \lambda_2 d_1 \boldsymbol{\gamma}_1 + \lambda_1 d_2 \boldsymbol{\gamma}_2}{\lambda_1 d_2 + \lambda_2 d_1} \cdot \nabla p$$



$$\lambda_i = \boldsymbol{n}_f \cdot \mathbb{K}_i \boldsymbol{n}_f$$

$$\boldsymbol{\gamma}_i = \mathbb{K}_i \boldsymbol{n}_f - \lambda_i \boldsymbol{n}_f$$

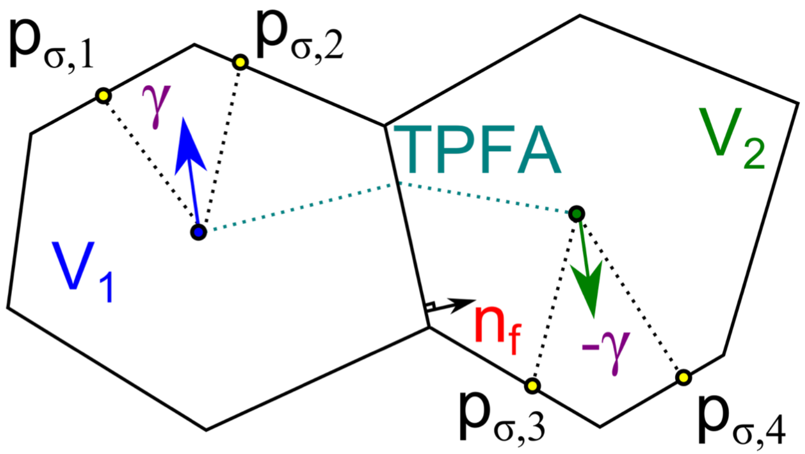
Terekhov, Mallison, Tchelepi “Cell-Centered Nonlinear Finite-Volume Methods for the Heterogeneous Anisotropic Diffusion Problem”, JCP 2017

Diffusion Problem

- Let us approximate these two parts using the formula:

$$q_{\tau,1} = \alpha_1\left(p_{\sigma,1} - p_1\right) + \alpha_2\left(p_{\sigma,2} - p_1\right),$$
$$-q_{\tau,2} = \beta_1\left(p_{\sigma,3} - p_2\right) + \beta_2\left(p_{\sigma,4} - p_2\right).$$

- Then the approximation of the missing part takes the form:



$$\begin{cases} q_\tau = \mu_1 q_{\tau,1} + \mu_2 q_{\tau,2} \\ \mu_1 + \mu_2 = 1 \end{cases}$$

Nonlinear convex combination

Positivity of the solution:

$$\mu_1 = \frac{\beta_1 p_{\sigma,3} + \beta_2 p_{\sigma,4}}{\beta_1 p_{\sigma,3} + \beta_2 p_{\sigma,4} + \alpha_1 p_{\sigma,1} + \alpha_2 p_{\sigma,2}}$$

$$\mu_2 = \frac{\alpha_1 p_{\sigma,1} + \alpha_2 p_{\sigma,2}}{\beta_1 p_{\sigma,3} + \beta_2 p_{\sigma,4} + \alpha_1 p_{\sigma,1} + \alpha_2 p_{\sigma,2}}$$

- Results in *M*-matrix with positive column sum

Discrete maximum principle:

$$\mu_1 = \frac{|q_{\tau,2}|}{|q_{\tau,1}| + |q_{\tau,2}|}$$

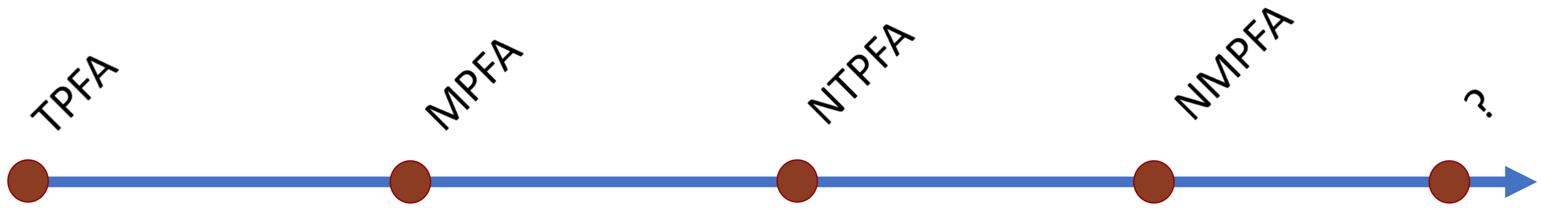
$$\mu_2 = \frac{|q_{\tau,1}|}{|q_{\tau,1}| + |q_{\tau,2}|}$$

- Results in *M*-matrix with positive row sum

Varga, “Iterative Matrix Analysis”, 1962
Stoyan, “On maximum principles for monotone matrices”, 1986

Overview

	TPFA	MPFA	NTPFA	NMPFA
Exact on Linear Solutions	NO!	YES	YES	YES
Small Stencil	YES	YES	YES	YES
Linear	YES	YES	NO	NO
Respect Maximum Principle	YES	NO	NO	YES
Efficiency	YES	YES	YES	NO



Linear Elasticity Problem

- In the absence of compressibility (otherwise tensor $\mathbb{C}$ is singular):

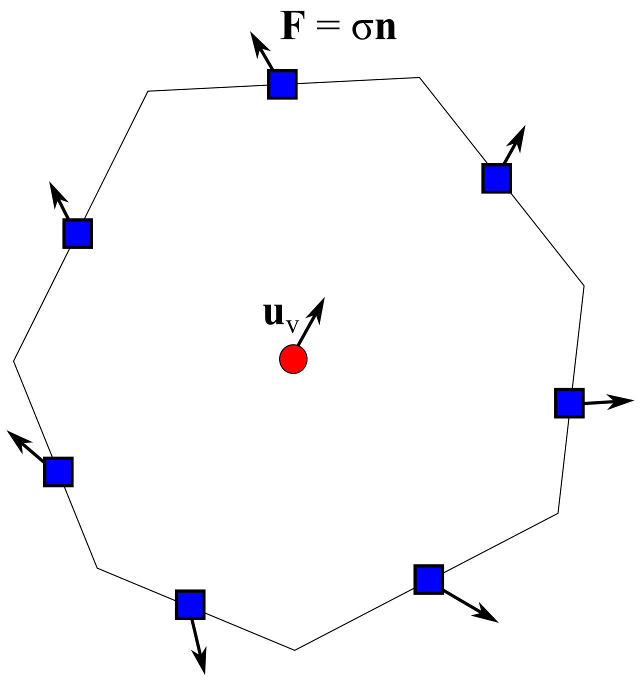
$$\mathbb{C}:\sigma\boldsymbol{n_f} = \frac{\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^{\mathrm{T}}}{2}\boldsymbol{n_f} \equiv \sigma\boldsymbol{n_f} = \mathcal{E}:\frac{\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^{\mathrm{T}}}{2}\boldsymbol{n_f} = \boldsymbol{F}$$

- In Voight notation matrix E is 6 by 6 equivalent of tensor $\mathcal{E}$, $\boldsymbol{\epsilon}$ is a vector of 6 components, equivalent to stress tensor:

$$\boldsymbol{F} = NE\boldsymbol{\epsilon}$$

- N – transformation of normal into 3 by 6 matrix:

$$N = \begin{pmatrix} n_x & & & & n_z & n_y \\ & n_y & & n_z & & n_x \\ & & n_z & n_y & n_x & \end{pmatrix}$$



Linear Elasticity Problem

- Transformations yield the flux expression, here $\mathbb{E}_{ij}$ are 3 by 3 tensors:

$$\boldsymbol{F} = N E \boldsymbol{\epsilon} = \begin{pmatrix} \mathbb{E}_{11}\boldsymbol{n_f} & \mathbb{E}_{12}\boldsymbol{n_f} & \mathbb{E}_{13}\boldsymbol{n_f} \\ \mathbb{E}_{12}^{\mathrm{T}}\boldsymbol{n_f} & \mathbb{E}_{22}\boldsymbol{n_f} & \mathbb{E}_{23}\boldsymbol{n_f} \\ \mathbb{E}_{13}^{\mathrm{T}}\boldsymbol{n_f} & \mathbb{E}_{23}^{\mathrm{T}}\boldsymbol{n_f} & \mathbb{E}_{33}\boldsymbol{n_f} \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \nabla u \\ \nabla v \\ \nabla w \end{pmatrix} = M \begin{pmatrix} \nabla u \\ \nabla v \\ \nabla w \end{pmatrix}$$

- New expression for $\boldsymbol{F}$ yields (as in **diffusion**):
  - *two-point flux*,
  - *transversal part* of the flux,
  - Interpolation method in *heterogeneous* media.

Linear Elasticity Problem

- **Two-point flux**, here $T_i = M_i(\mathbb{I} \otimes \boldsymbol{n}_f)$ - matrix 3 by 3:

$$\boldsymbol{F}_\mathrm{n} = \underline{T_1(d_1 T_2 + d_2 T_1)^{-1} T_2}(\boldsymbol{u}_2 - \boldsymbol{u}_1)$$

Tensorial harmonic average

- Lost **transversal correction**:

$$\boldsymbol{F}_\tau = \begin{pmatrix} T_1(d_1 T_2 + d_2 T_1)^{-1} T_2\left(\mathbb{I} \otimes (\boldsymbol{y}_2 - \boldsymbol{y}_1)^\mathrm{T}\right) \\ +d_1 T_2 (d_1 T_2 + d_2 T_1)^{-1}\left(M_1 - T_1\left(\mathbb{I} \otimes \boldsymbol{n}_f^\mathrm{T}\right)\right) \\ +d_2 T_1 (d_1 T_2 + d_2 T_1)^{-1}\left(M_2 - T_2\left(\mathbb{I} \otimes \boldsymbol{n}_f^\mathrm{T}\right)\right) \end{pmatrix} \begin{pmatrix} \nabla u \\ \nabla v \\ \nabla w \end{pmatrix}$$

- Scheme is applicable on **general grids** with **full anisotropic** tensors.

Terekhov, Tchelepi "Cell-centered finite volume method for heterogeneous full-tensor anisotropic linear elasticity", submitted to CMAME

Incompressible Navier-Stokes

- Flux expression:

$$\boldsymbol{F} = \begin{cases} \rho \boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{n_f} - \mu\nabla\boldsymbol{u}\boldsymbol{n_f} + p\boldsymbol{n_f} \\ \boldsymbol{n_f}^{\mathrm{T}}\boldsymbol{u} \end{cases}$$

- Key part for stabilization is the analysis of the system:

$$\boldsymbol{F}_{\boldsymbol{GD}} = \begin{cases} p\boldsymbol{n_f} \\ \boldsymbol{n_f}^{\mathrm{T}}\boldsymbol{u} \end{cases} = \begin{pmatrix} & \boldsymbol{n_f} \\ \boldsymbol{n_f}^{\mathrm{T}} & \end{pmatrix} \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} = \frac{1}{2}\begin{pmatrix} \boldsymbol{n_f}\boldsymbol{n_f}^{\mathrm{T}} & \boldsymbol{n_f} \\ \boldsymbol{n_f}^{\mathrm{T}} & 1 \end{pmatrix} \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} + \frac{1}{2}\begin{pmatrix} -\boldsymbol{n_f}\boldsymbol{n_f}^{\mathrm{T}} & \boldsymbol{n_f} \\ \boldsymbol{n_f}^{\mathrm{T}} & -1 \end{pmatrix} \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix}$$

Positive and negative eigenvalues — Positive eigenvalue — Negative eigenvalue

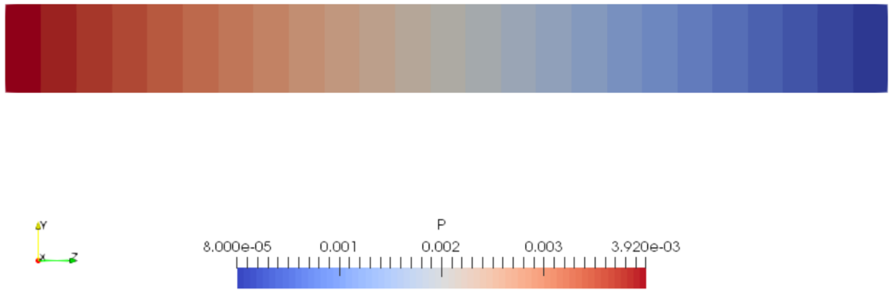
- Accurate (*nonlinear*) approach to approximation removes oscillations.

Terekhov, Vassilevski, "On A Finite-Volume Method For Saddle-Point Problems", Submitted to JCP
Terekhov, Vassilevski "Stable collocated finite-volume method for incompressible Navier-Stokes equations", In preparation

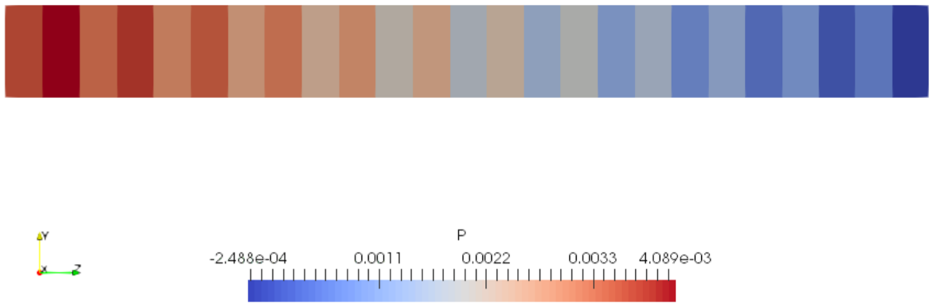
Incompressible Navier-Stokes

- Poiseuille flow:

Positive-definite div-grad



Direct approximation of div-grad



- Demonstrates **second-order convergence** on Ethier-Steinman problem, error norms are comparable to projection scheme on staggered grid (MAC-scheme).

Thank you for Attention!

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