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Institute of Computational Science ICS

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Center for Computational Medicine in Cardiology CCMC
Institute of Computational Science ICS
Faculty of Informatics

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SWISS COMPETENCE CENTER for ENERGY RESEARCH
SUPPLY of ELECTRICITY

FNSNF
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SCHWEIZERISCHER NATIONALFONDS
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SWISS NATIONAL SCIENCE FOUNDATION

Eurohack 2018
Utopia an EDSL for scientific computing

Team: Patrick Zulian, Alena Kopanicakova, Maria Nestola, Nur Fadel, Andreas Fink

Mentors: Carter Edwards (NVIDIA), Christian Trott (SNL)

NVIDIA

Sandia National Laboratories

October 2nd, 2018, Lugano

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

Introduction

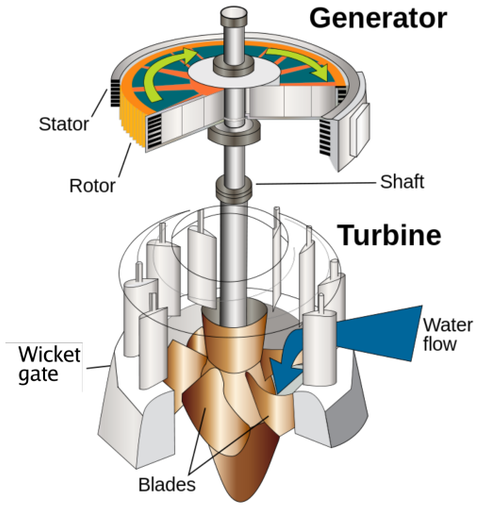
High-performance computing

Usability

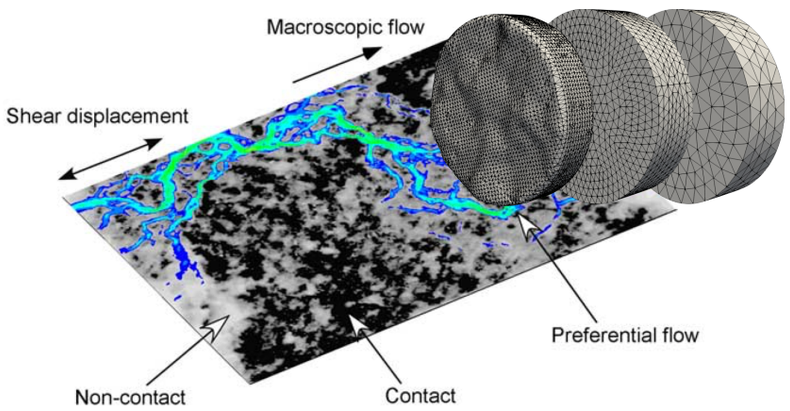
+

Flexibility!

Computational energy



Water turbines



Computational Geophysics

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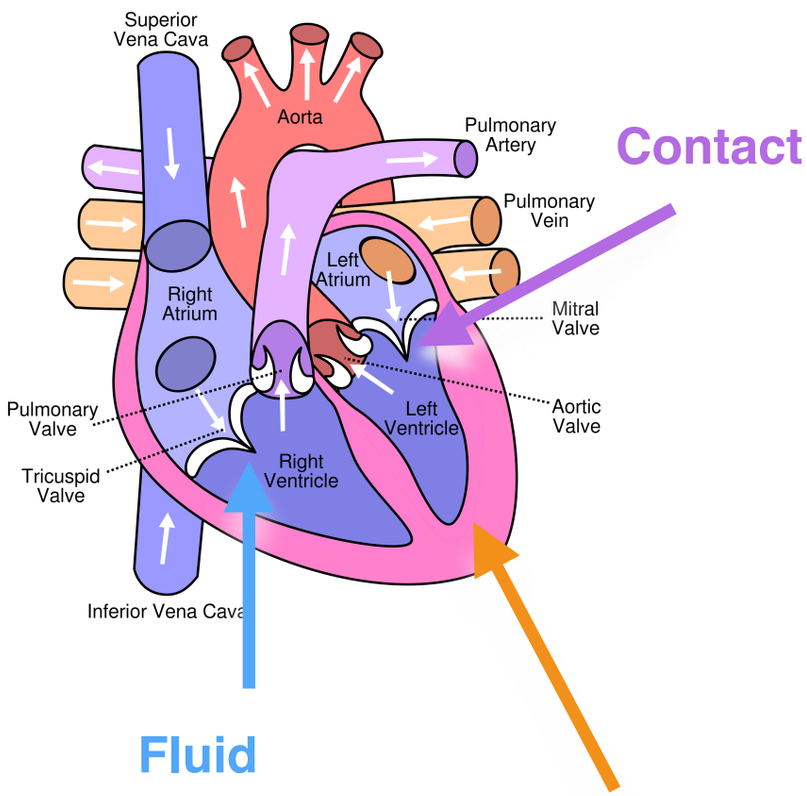
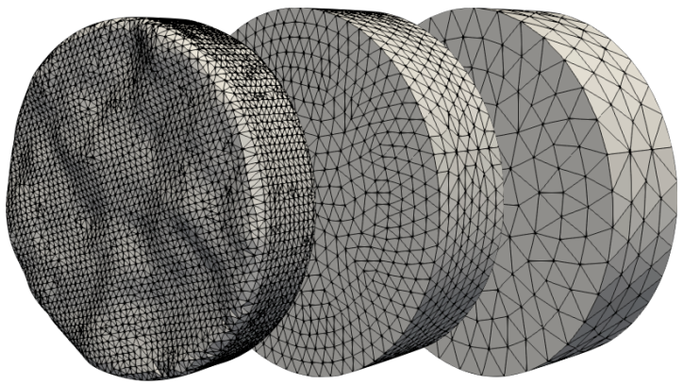
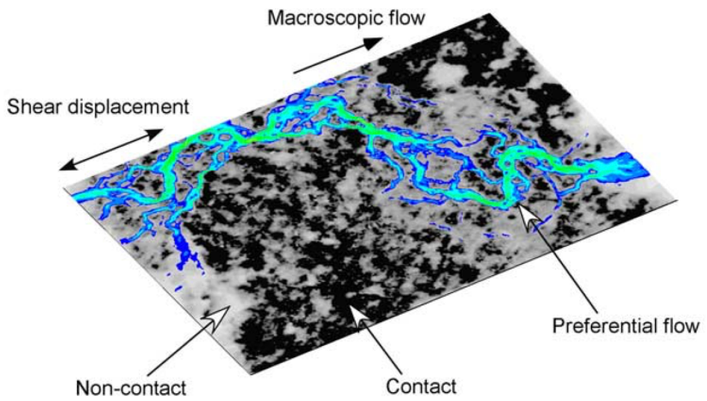
Other applications

Simulation of the heart

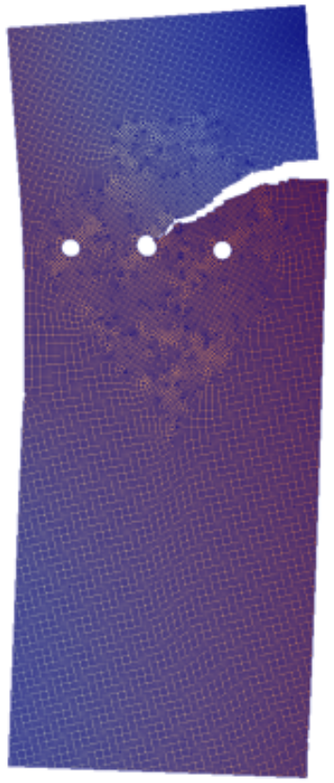


Multilevel solution methods

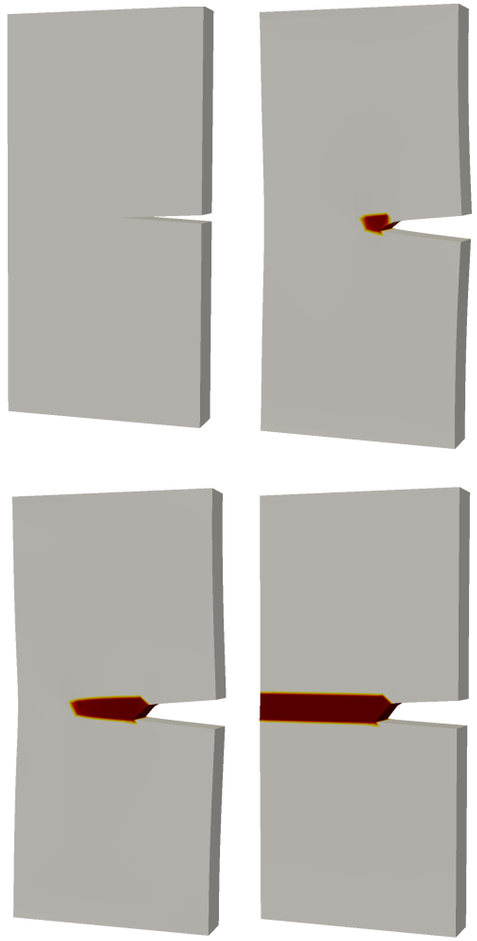




Multigrid solver for **computational geology** (C. Von Planta)



Multigrid solver for **crack simulations** with XFEM[1] (H. Kothari)



Multigrid solver for **Phase-field method**[2] (A. Kopaničáková)

Literature: **1** Z. Goangseup, and T. Belytschko, 2003.
2 C. Miehe, F. Welschinger, and M. Hofacker, 2010.

Example utopia code (Neo-hookean material Hessian and gradient)

```
auto mu     = params_.var_mu();
auto lambda = params_.var_lambda();

auto u  = trial(V_);
auto v  = test(V_);
auto uk = interpolate(x, u);

auto F       = identity() + grad(uk);
auto F_t     = transpose(F);
auto F_inv   = inv(F);
auto F_inv_t = transpose(F_inv);
auto J       = det(F);

auto P = mu * (F - F_inv_t) + (lambda * logn(J)) * F_inv_t;

auto stress_lin = mu * grad(u)
-(lambda * logn(J) - mu) * F_inv_t * transpose(grad(u)) * F_inv_t
+ inner(lambda * F_inv_t, grad(u)) * F_inv_t;

auto l_form = inner(P, grad(v)) * dX;
auto b_form = inner(stress_lin, grad(v)) * dX;
```

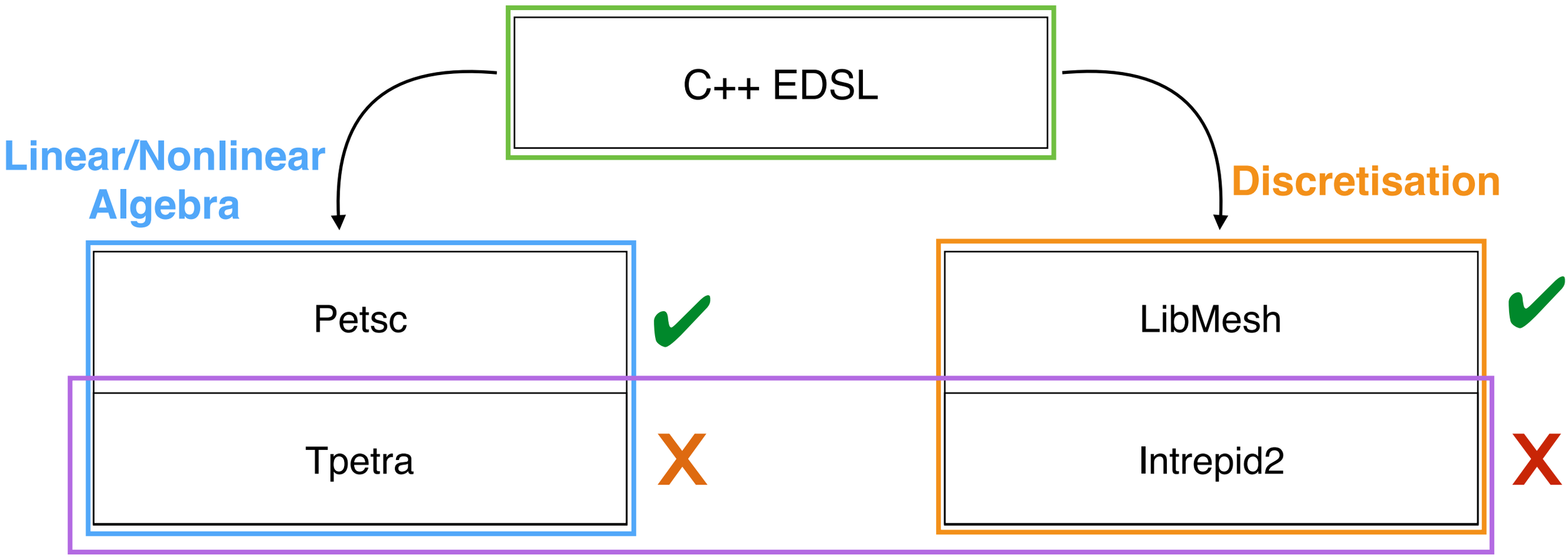
Front-end

```
assemble(b_form == l_form, hessian, gradient);
```

Back-end

Overview

Architecture



Goal for the hackathon

GPU porting approach and status

Approach

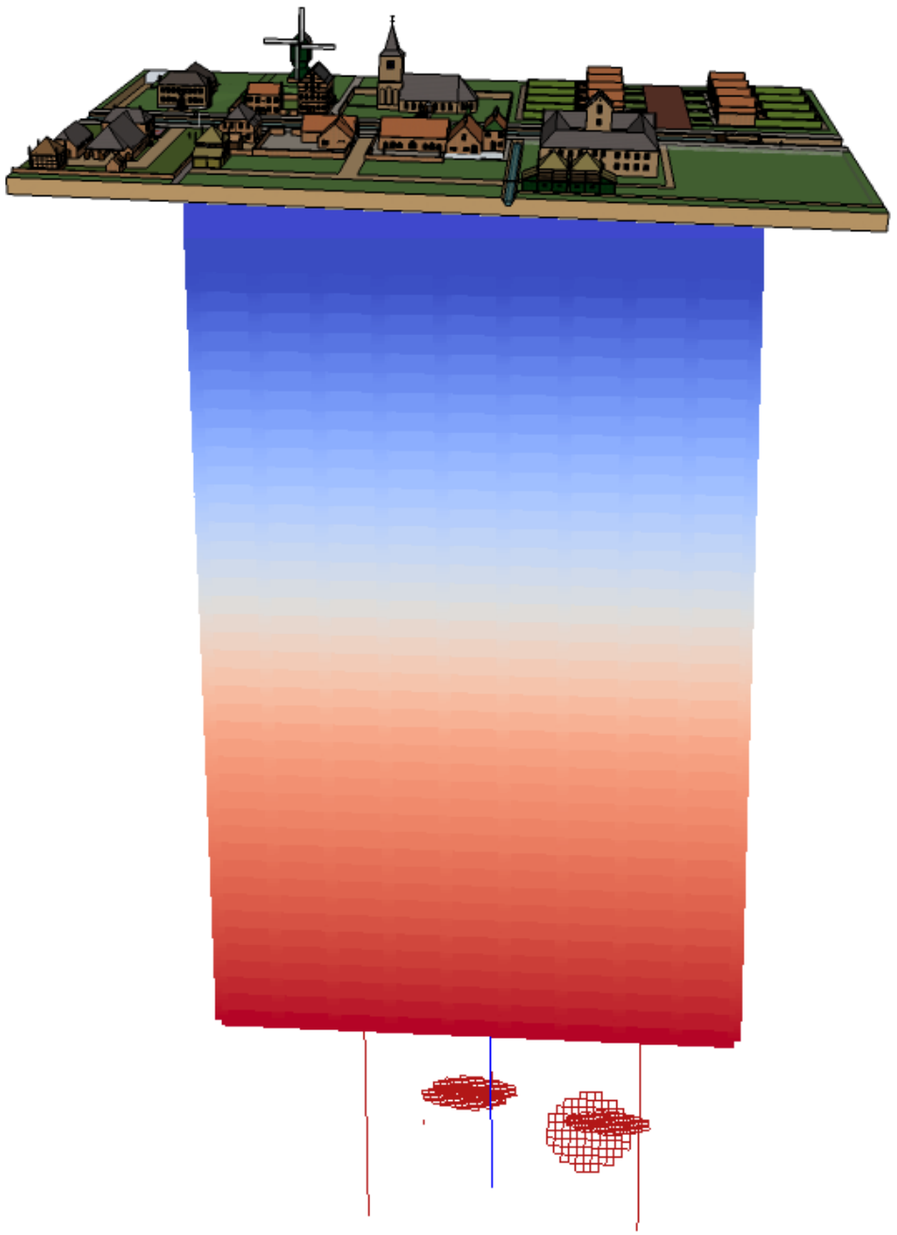
- Exploit existing functionalities from Trilinos (**Tpetra** and **Intrepid2**)
- Implementing missing functionalities with **Kokkos**

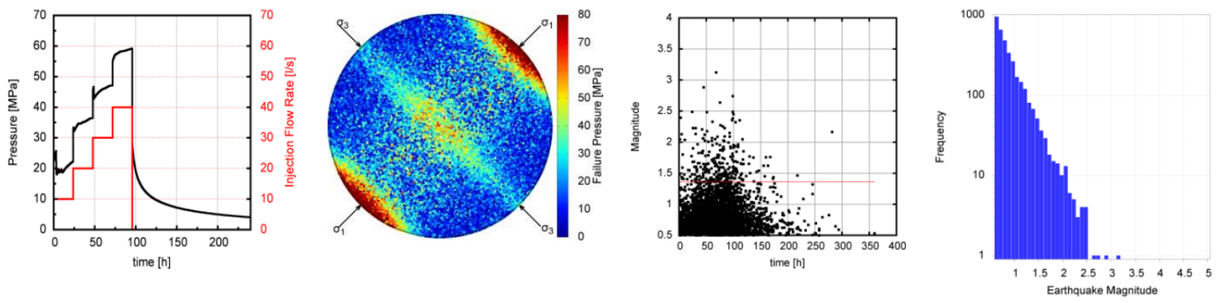
Status

- Basic **Tpetra** backend implemented with still few bugs
- Integration of **Intrepid2** has to be done from scratch

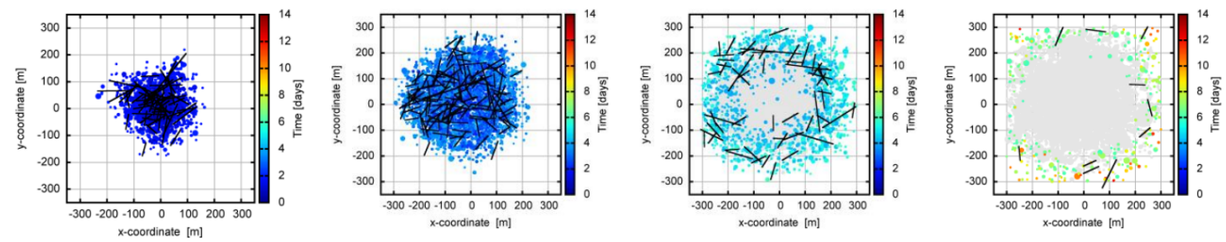
Plan (FASTER)

- Profile of FASTER with utopia and optimise it for the least overhead possible (**Andreas**)

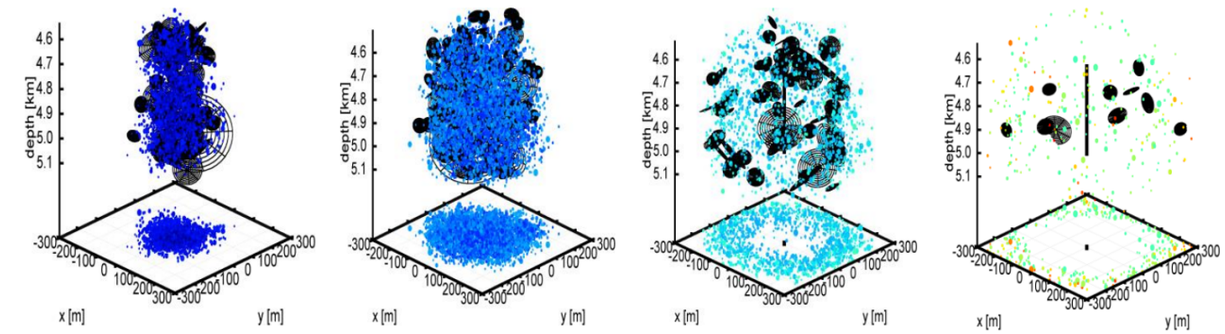




(a) (b) (c) (d)



(e) 0-2 days (f) 2-4 days (g) 4-6 days (h) 6-14 days



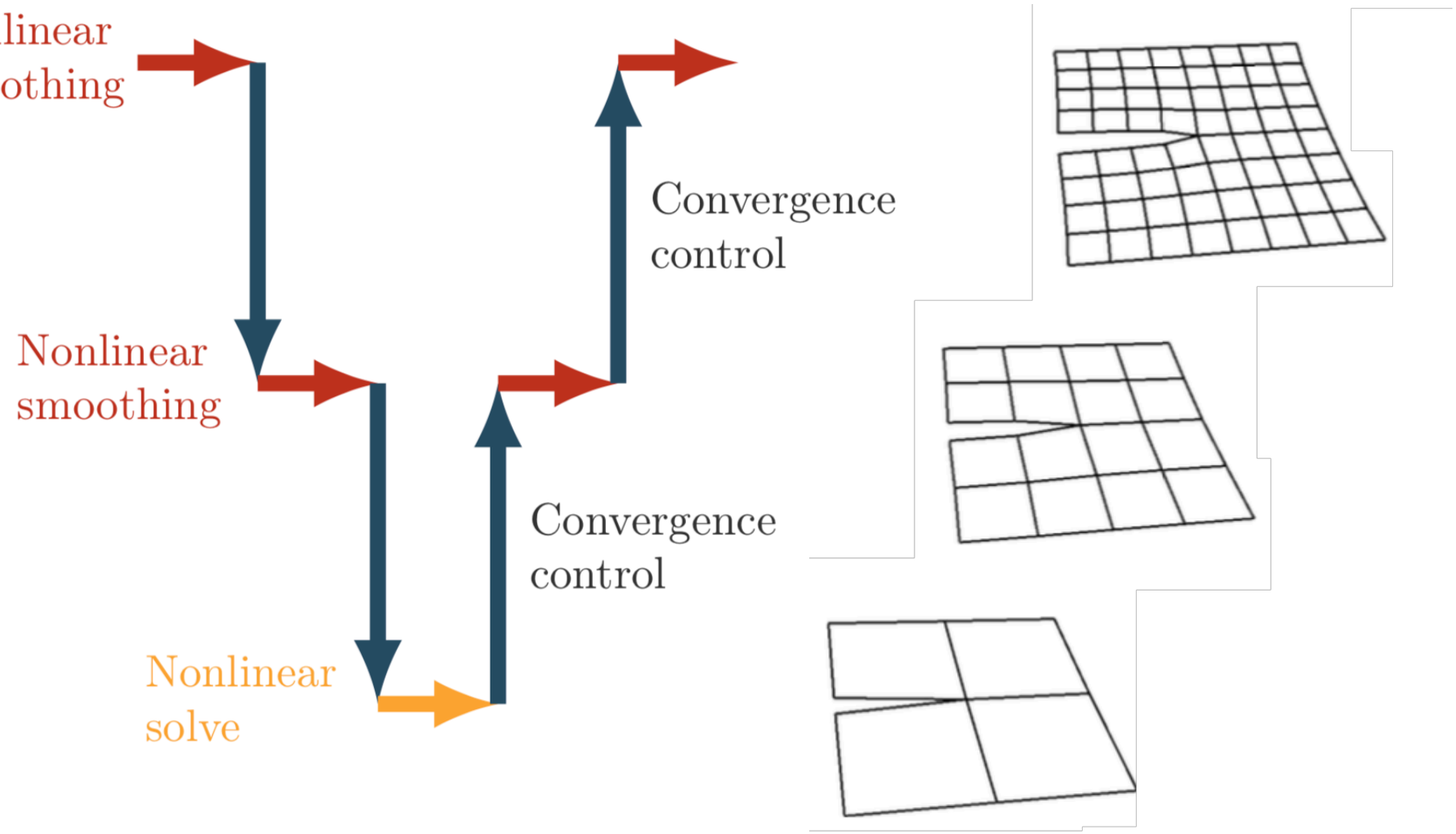
(i) 0-2 days (j) 2-4 days (k) 4-6 days (l) 6-14 days

Plan (Utopia algebra)

- Implement all *TODOs* for the tpetra-backend (**Maria**, **Patrick**, **Nur**)
  - Fix transpose operations for rectangular matrices
  - Fix ghost value handling for fe
  - Implement operations that are missing in tpetra using kokkos
  - Find performance bugs and fix them

Plan (RMTR)

- Recursive Multilevel Trust Region aka RMTR (Alena)
  - Make implementation robust
  - Profile, find bottlenecks, improve, profile,…
  - Compare performance against petsc version



Plan (Utopia FE)

- Proof of concept for utopia_fe for new backend with Intrepid2 (Patrick/Nur)
  - Re-factor code for allowing new backend usage
  - Laplace equation

```
auto u   = trial(V);
auto v   = test(V);
auto b_form = inner(grad(u), grad(v)) * dX;
utopia::assemble(b_form, H);
utopia::assemble(inner(coeff(1.), v) * dX, rhs);
```