Computational Frameworks enabling multi-scale multi-physics models

Elizabeth & Frederick White Conference

Mastering the Data Explosion in the Earth and Environmental sciences

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Outline

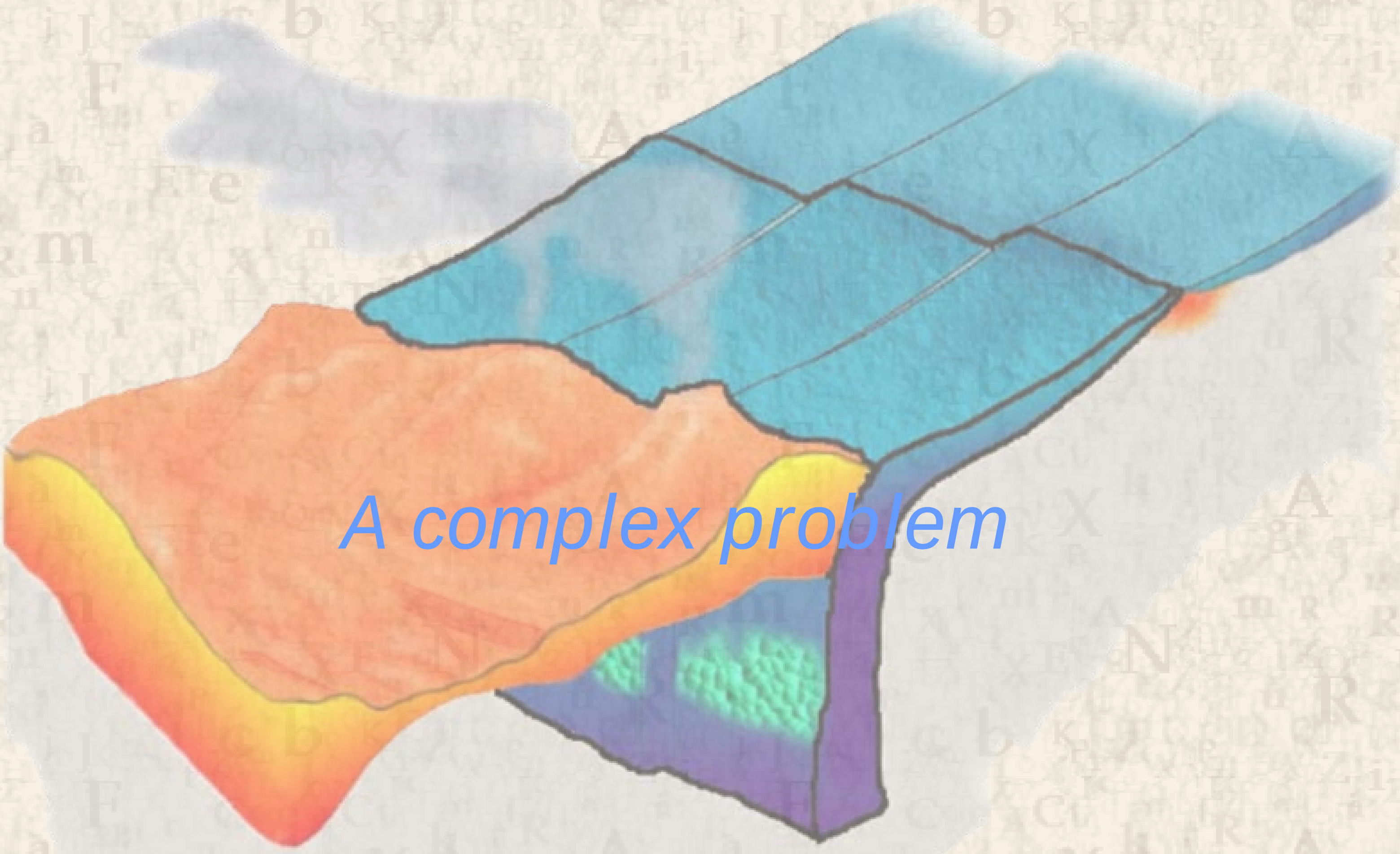
- *Why computational frameworks?*
  - *And what does that have to do with information explosions?*
- *Our computational framework*
  - *A cooks tour*
- *Where to from here*

Why Computational Frameworks

- *Increasing Quality and Quantity of Data*
  - *Allows us to develop and test ever more accurate models of the evolution of the earth*
    - *For vastly more model runs*
  - *Data has no value unless it is turned into information*
- *Traditional computer modeling*
  - *2D models, fixed format input*
  - *Hand-written hero codes*
- *We need a way to construct far more flexible computer models - frameworks*

Why Computational Frameworks (cont.)

- *Frameworks are everywhere in commercial software: .NET and J2EEE*
- *What do they BUY you in geophysics? Reuse!*
  - *Coupling*
    - *Models share coupling components & techniques*
  - *Data logging (model archives) components*
  - *Visualization*
    - *Glucifer in our framework*
  - *Grid computing*



A complex problem

Long term geodynamics

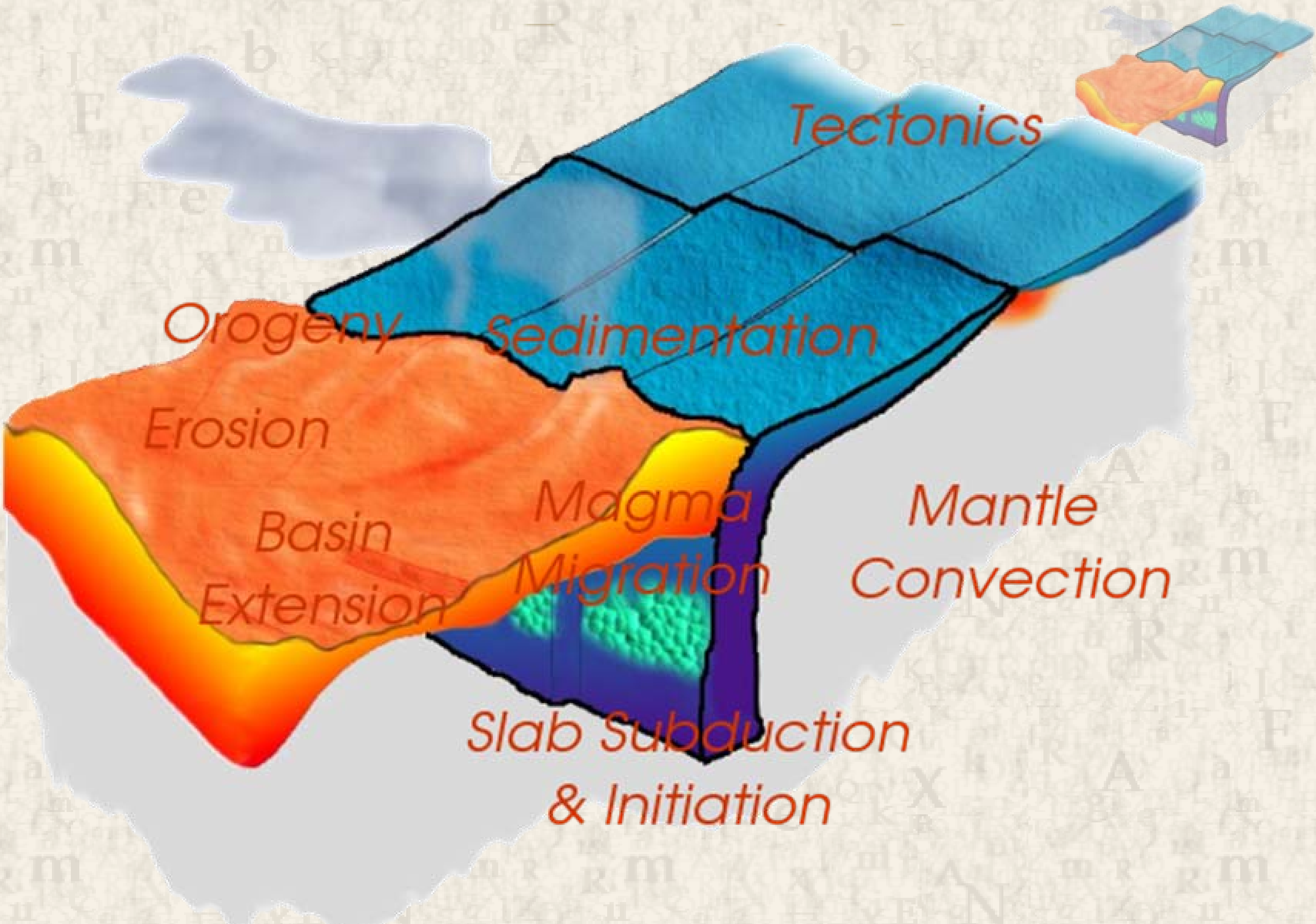
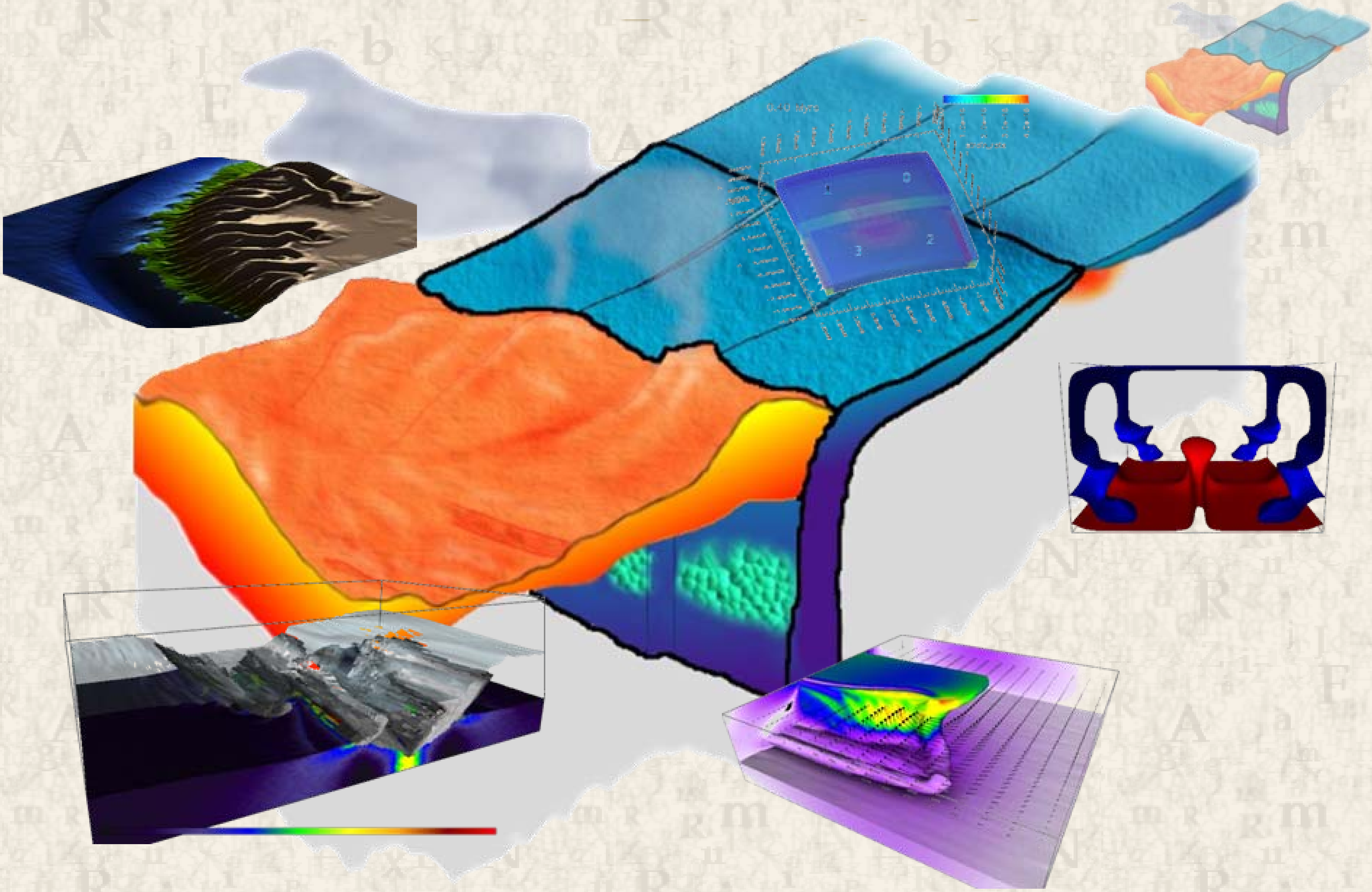


Image courtesy of Professor Louis Moresi

Codes that simulate these processes

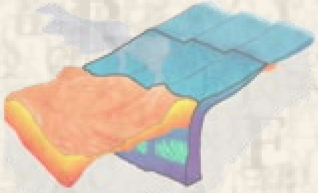


Rephrase: …“almost simulate”…

Each of these long term geophysics processes fail to reliably and truthfully simulate their respective parts of the Earth…

- *The Earth is complex, with (what we assume as) these processes interacting with each other*
- *These codes have constrained scope of signals*
  - *We make assumptions of behaviour at smaller/larger scales*
  - *We make assumptions of behaviour at process boundaries*
- *It is difficult to validate models*
  - *Can’t go build an Earth in a lab*
  - *Its an inverse problem*
    - *We potentially have data for today,*
    - *The codes start from the past*

Assumptions



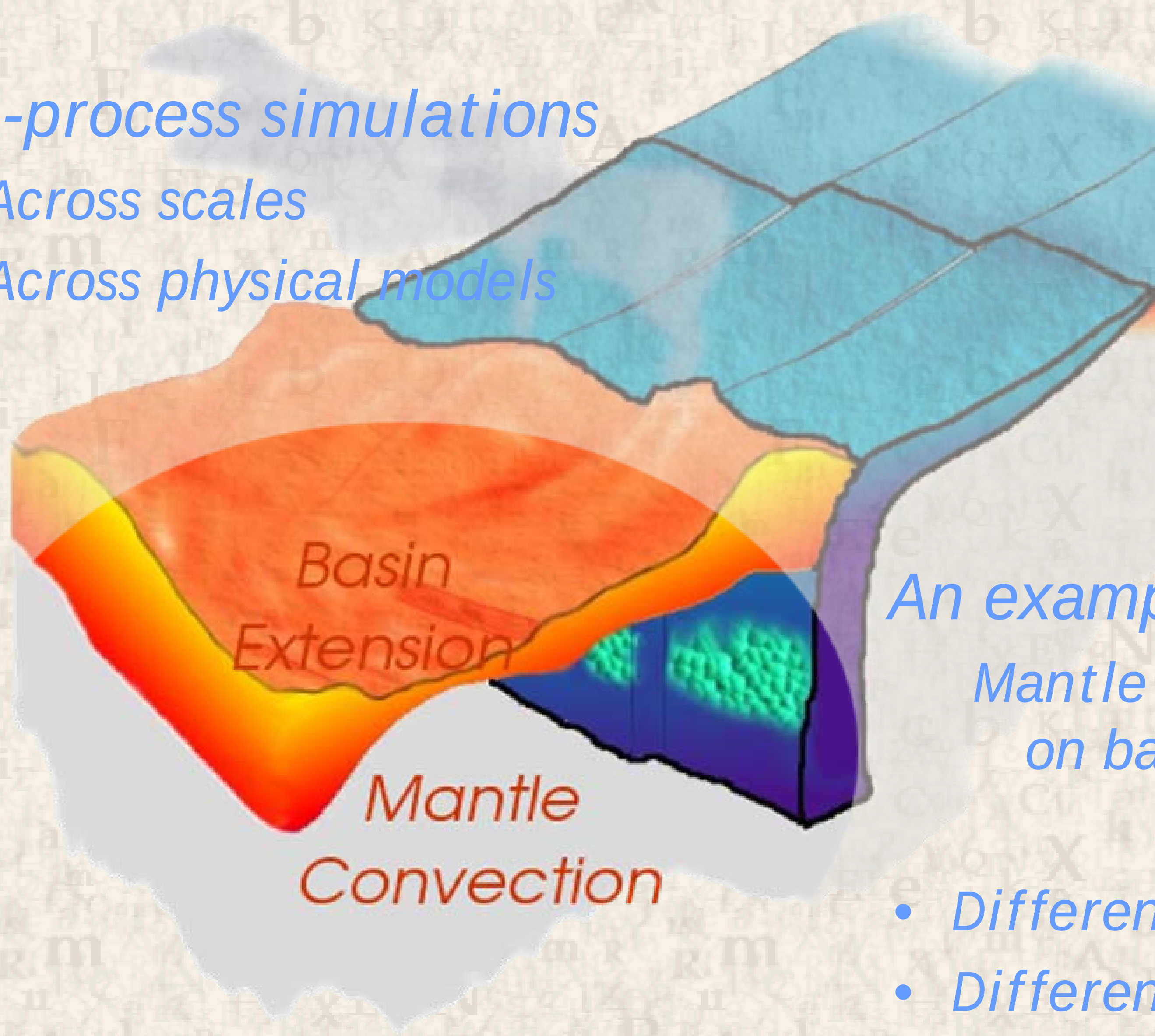
- *We make these (scale/boundary) assumptions to deal with:*
  - *Complexity of the model*
  - *Time to run the model*

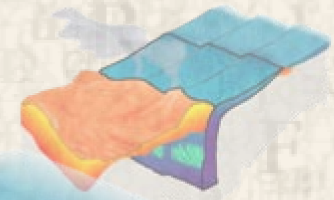
- *As a consequence, codes have numerics optimised for its scale and structures adequate for its physics*

The emerging need…

Multi-process simulations

- *Across scales*
- *Across physical models*





An example:

Mantle influences on basin models

- *Different numerics*
- *Different physics*

Evolving to multi-process problems

In practice, changing a code's numerics and physics is difficult because they significantly influences low-level coding structures

Either...

- *Take existing solutions/codes, and couple them together*
- *Create a framework that enables interchangeability of and encourages development of the necessary numerics and physics*

Can we be in a position to solve it either way?

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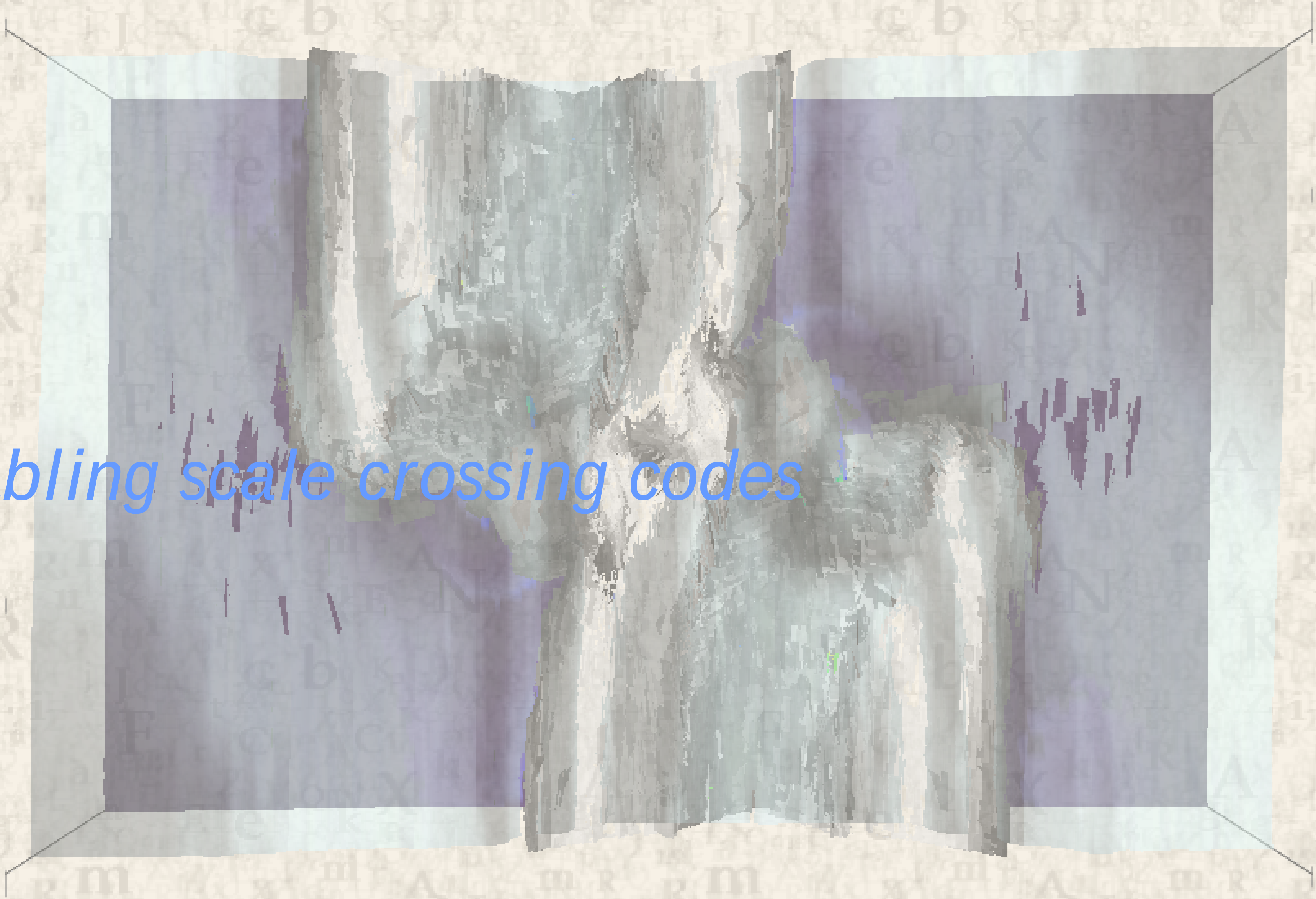
Enabling scale crossing codes



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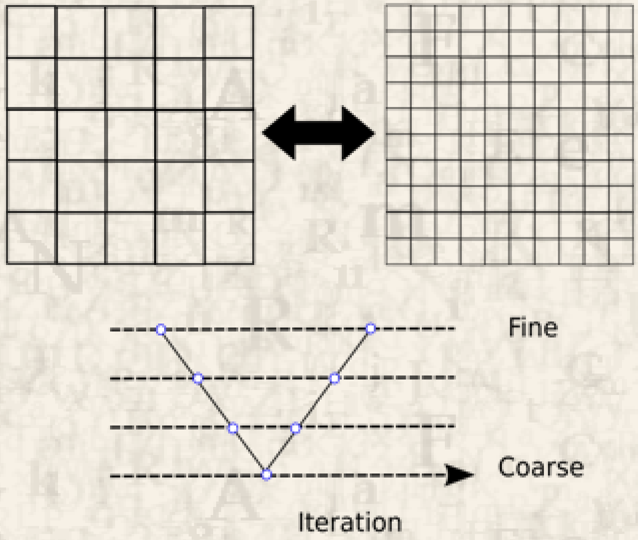
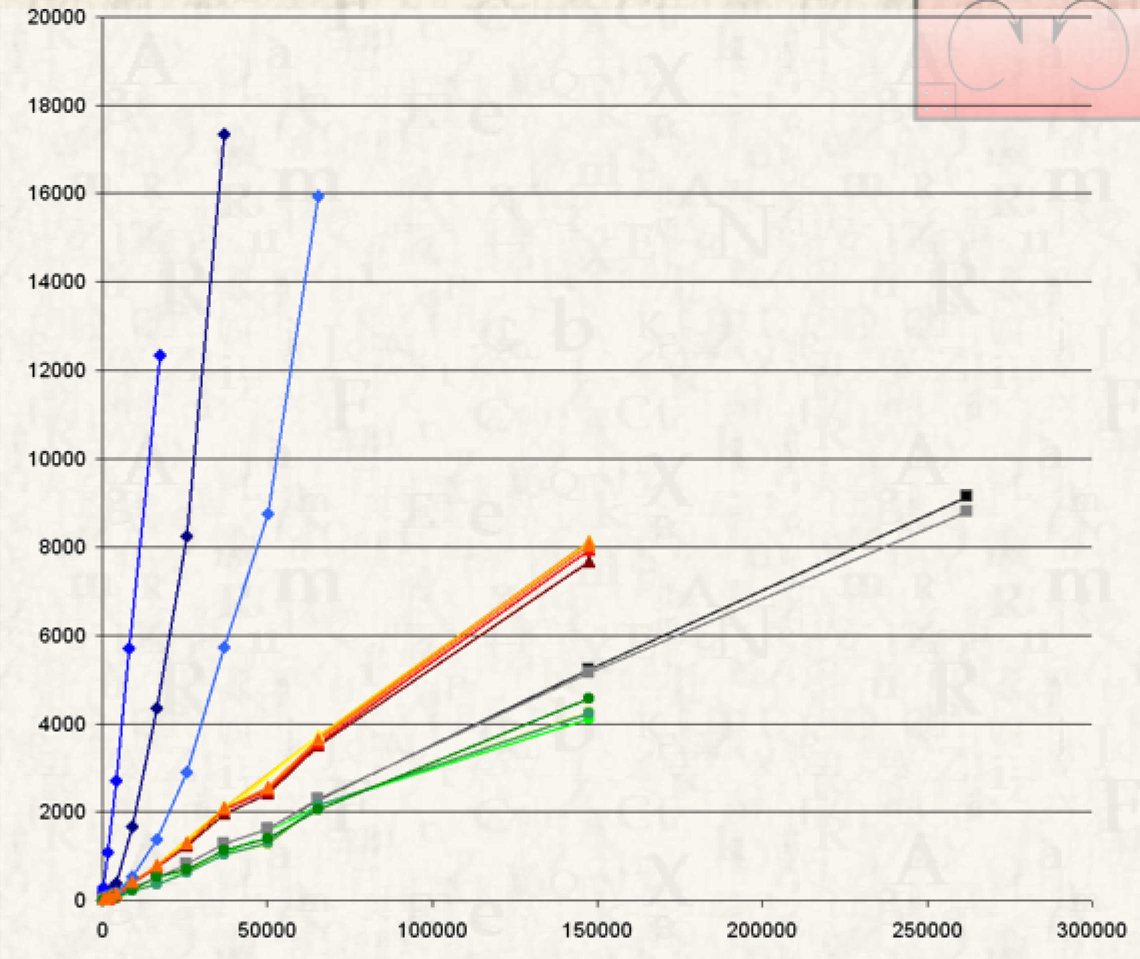
Multigrid



- *With Multigrid, you effectively solve the same problem at numerous coarseness levels*
  - *Separate linear systems*
  - *We couple by residuals*

Multigrid scaling

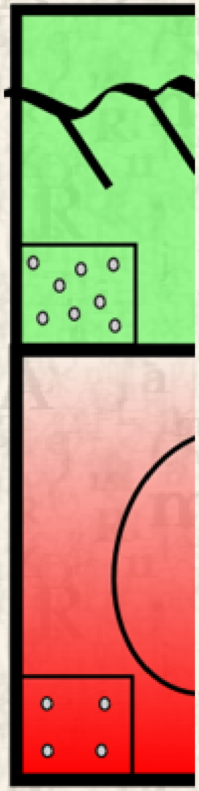
- *The problem with (most) Finite Element codes is that they rely on building large systems of linear equations that must be solved either:*
  - *Exactly / Directly ~O(C*U³)*
  - *Approximately / Iterative O(K*U<3), K>C*
- *Result: finer meshes (and use more processors) are useless because it just takes too long!*
- *Multigrid - scales ~linearly to unknowns*
  - *Very problem specific*
  - *Needs more memory*

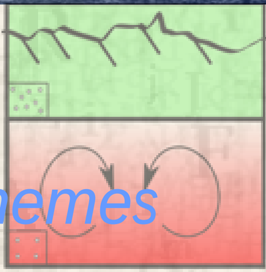


Adaptive Mesh Refinement

- *We don't do it… yet.*
- *Allows one to start with a coarse, large area. The domain refines in areas where more accuracy is needed*
  - *Can turn on/off appropriate physics in different parts of the domain*
- *Benefits:*
  - *Continuous domain*
  - *Accurate*
- *Problems:*
  - *Not easy load balance in parallel – no freely available tools to help*

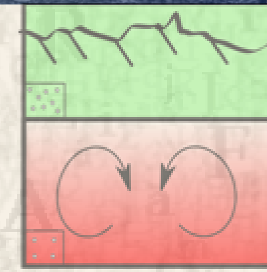
PICellerator



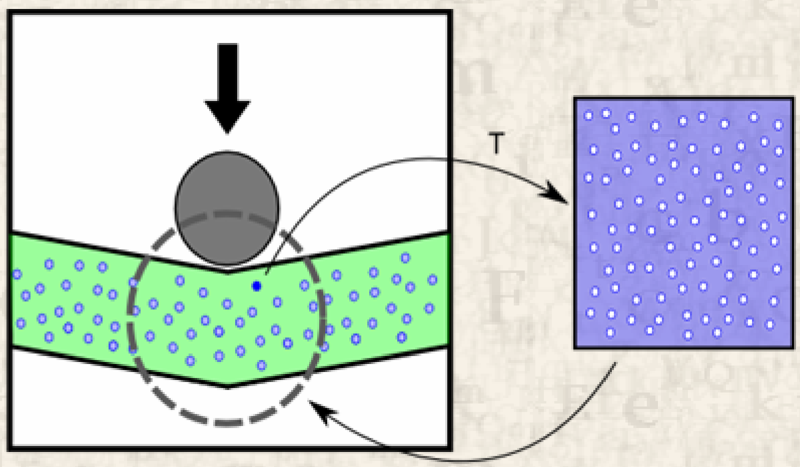


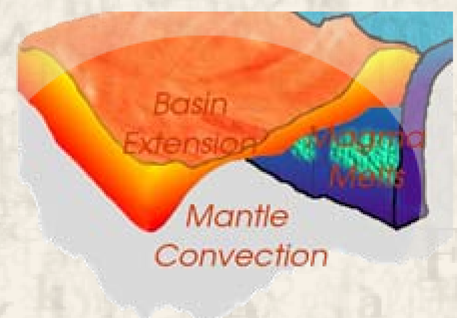
- *Framework for Lagrangian Integration schemes*
- *Presently has PIC*
  - *Material "are" integration points - coincidence*
  - *Brilliant where material histories are important*
- *Under development*
  - *Material points and integration points are not the same*
    - *E.g. Integration moves to reduce error, material advects with the material flow*
  - *Hybrids*
    - *Gaussian (standard FEM) is the cheapest (memory & time)*

Representative volumes



- *Homogenisation by representative volumes*
- *Have different physics models at two distinct scales*
- *The macro (larger) scale's constitutive behaviour for a certain sub-domain is evaluated by a representative volume (micro)*
- *Potential huge memory and load, but conceptually clear multi-scale*





Where to from here?

- *Our frameworks are public domain and open source*
  - *www.csd.vpac.org*
  - *Dozens of active users/developers*
  - *But they will succeed only if there is a community behind them (users and developers)*
- *Increasing international collaboration/users*
  - *Especially with the USA, the Centre for Computational Infrastructure (CIG)*
  - *www.geodynamics.org*