A Discontinuous Galerkin Method for the Advection of non-Diffusive Fields in Solid Earth Geodynamics: Demonstration and Comparison with Other Methods in the Mantle Convection Code ASPECT

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Oct 16, 2016 @ College of Earth Sciences,
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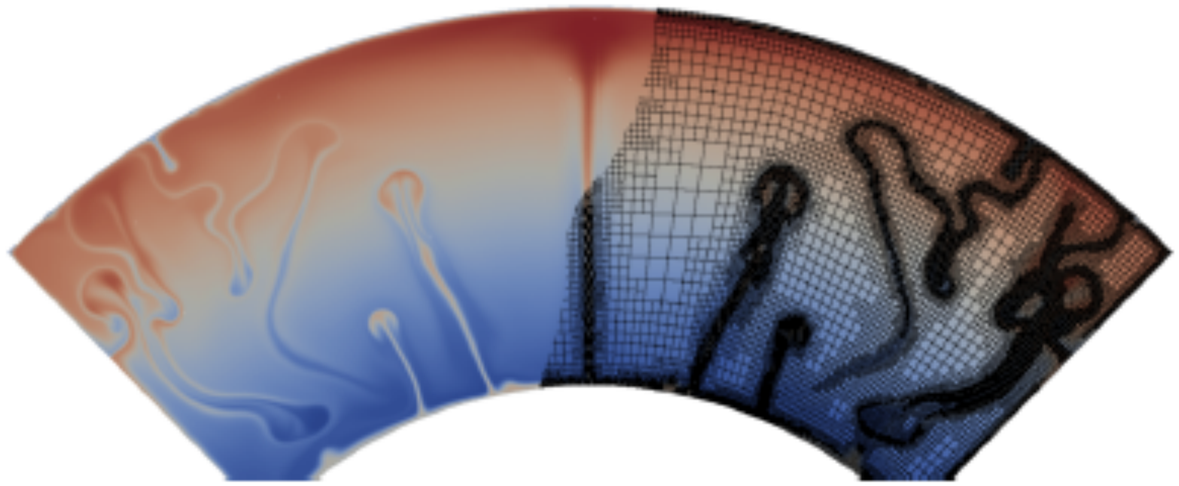
Outline

- Introduction of ASPECT
- Discontinuous Galerkin method with a bound preserving limiter method for the Advection of non-Diffusive Fields in Solid Earth Geodynamics
- Numerical experiments
- Conclusions

Part I
Introduction of ASPECT

What?

ASPECT = **A**dvanced **S**olver for **P**roblems in **E**arth's **C**onvec**T**ion



- Mantle convection using modern numerical methods
- Open source, C++
- Available at: `http://aspect.dealii.org`
- Supported by NSF/CIG:

National Science Foundation
WHERE DISCOVERIES BEGIN

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Kronbichler, Heister and Bangerth.
High Accuracy Mantle Convection Simulation through Modern Numerical Methods.
Geophysical Journal International, 2012, 191, 12-29.

Who?

- Wolfgang Bangerth, Timo Heister
- Contributors (total: 31):
  Jacky Austermann, Eva Bredow, Markus Bürg, Sam Cox, Juliane Dannberg, William Durkin, Grant Euen, René Gaßmöller, Thomas Geenen, Anne Glerum, Ryan Grove, Menno Fraters, Ying He, Eric Heien, Lorraine Hwang, Louise Kellogg, Martin Kronbichler, Shangxin Liu, Kimee Moore, Elvira Mulyukova, Bob Myhill, John Naliboff, Sanja Panovska, Jonathan Perry-Houts, Elbridge Gerry Puckett, Ian Rose, Max Rudolph, Benjamin Smith, Sarah Stamps, Scott Tarlow, Cedric Thieulot, Bruno Turcksin, Iris van Zelst, Siqi Zhang

Timeline

- 2008-2011: deal.II based examples/experiments (Bangerth)
- Oct 2011: Aspect development started
- March 2012: release 0.1
- April 2013: release 0.2
- May 2013: release 0.3 (bugfixes)
- April 2014: release 1.0
- June 2014: release 1.1
- January 2015: release 1.2
  solver improvements, concentric shells, boundary names, plugins, ...
- May 18 2015: release 1.3
  material averaging, nullspace handling, output grouping, ascii data, stress postprocessing, ...
- May 15 2016: release 1.4
  Particle overhaul, modularizing assembly, flexible FEM variables, heating models, DG, signals, . . .

ASPECT as software:
Philosophy and numerical methods

Codes in Geodynamics

- There are some widely used codes
- Almost all codes use globally refined meshes
- Almost all codes use lowest order elements
- Most codes use "simple" solvers
- No code has been "designed" with a view to
  – extensibility
  – maintainability
  – correctness

Geodynamics: Design challenges

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

As a "community code", *Aspect* needs to satisfy these goals:

- Can solve problems of interest (to geodynamicists)
- Be well tested
- Use modern numerical methods
- Be very easy to extend to allow for experiments
- Freely available

Equations

$$-\nabla \cdot \left[2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) \right] + \nabla p = \rho \mathbf{g}$$

Momentum equation

Divergence of stress tensor

Pressure gradient

Gravity force

Only viscous stress (no elasticity/plasticity), no inertia

(Total pressure instead of only dynamic pressure)

$\mathbf{u}$	velocity	$\frac{m}{s}$
p	pressure	Pa
T	temperature	K
$\varepsilon(\mathbf{u})$	strain rate	$\frac{1}{s}$
η	viscosity	$\mathrm{Pa} \cdot \mathrm{s}$

ρ	density	$\frac{kg}{m^3}$
$\mathbf{g}$	gravity	$\frac{m}{s^2}$
C_p	specific heat capacity	$\frac{J}{kg \cdot K}$
k	thermal conductivity	$\frac{W}{m \cdot K}$
H	intrinsic specific heat production	$\frac{W}{kg}$

Equations

$$-\nabla \cdot \left[2\eta\left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right)\right] + \nabla p = \rho \mathbf{g}$$

Momentum equation

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

Conservation of mass

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) - \nabla \cdot k \nabla T = \rho H$$
$$+ 2\eta\left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right)$$
$$-\frac{\partial \rho}{\partial T} T \mathbf{u} \cdot \mathbf{g} \quad + \rho T \cdot \Delta S \frac{DX}{Dt}$$

Conservation of energy

$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = 0$$

Advection of compositional fields

Field method (or tracer method)

Summary of equations

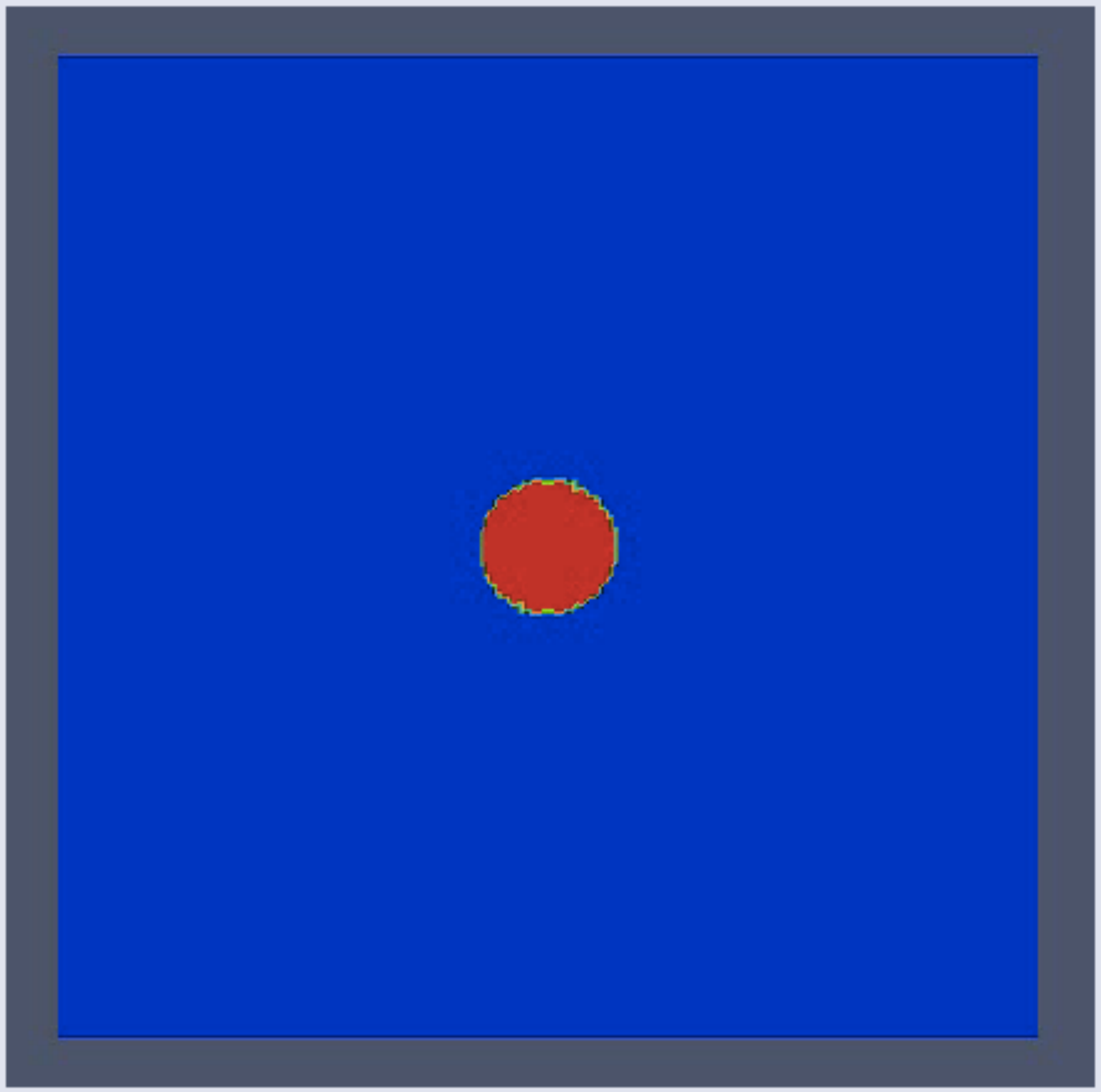
- Compressibility
- 2- or 3-dimensional domain Ω, different geometries
- Total pressure
- Radiogenic heating
- Adiabatic heating, shear heating & latent heat
- Advection of any number of compositional fields

Numerical methods

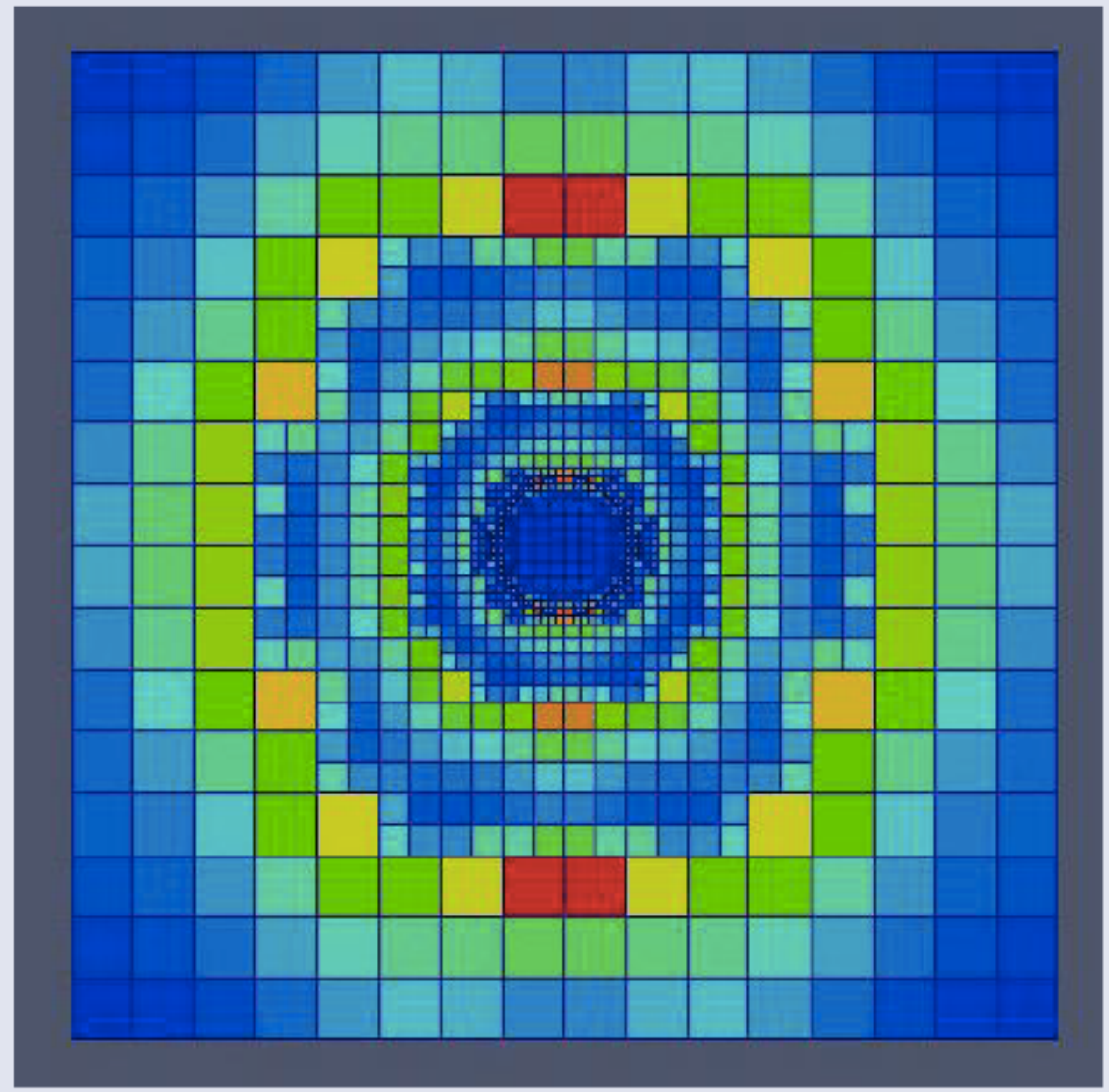
- Mesh adaptation
- Accurate discretizations (choice of finite element for velocity and pressure + nonlinear artificial diffusion for temperature stabilization)
- Efficient linear solvers (preconditioner + algebraic multigrid)
- Parallelization of all of the steps above
- Modularity of the code

Mesh adaptation

- Example: Composition as refinement strategy



Compositional field



Mesh cells, colors indicate the estimated error

Mesh adaptation

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Choose **Strategies**:
temperature, density, velocity, composition, thermal energy density

Calculate error estimate c_K (based on 2nd derivatives & cell diameter)

$$E = \sum_{K \in T} c_K$$

Total error estimate E

Normalize refinement criteria?

Scale errors for each criterium?

Add errors/take maximum?

Choose **refinement + coarsening fraction** ***a***

Look for the smallest subset M

$$aE = \sum_{K \in M} c_K$$

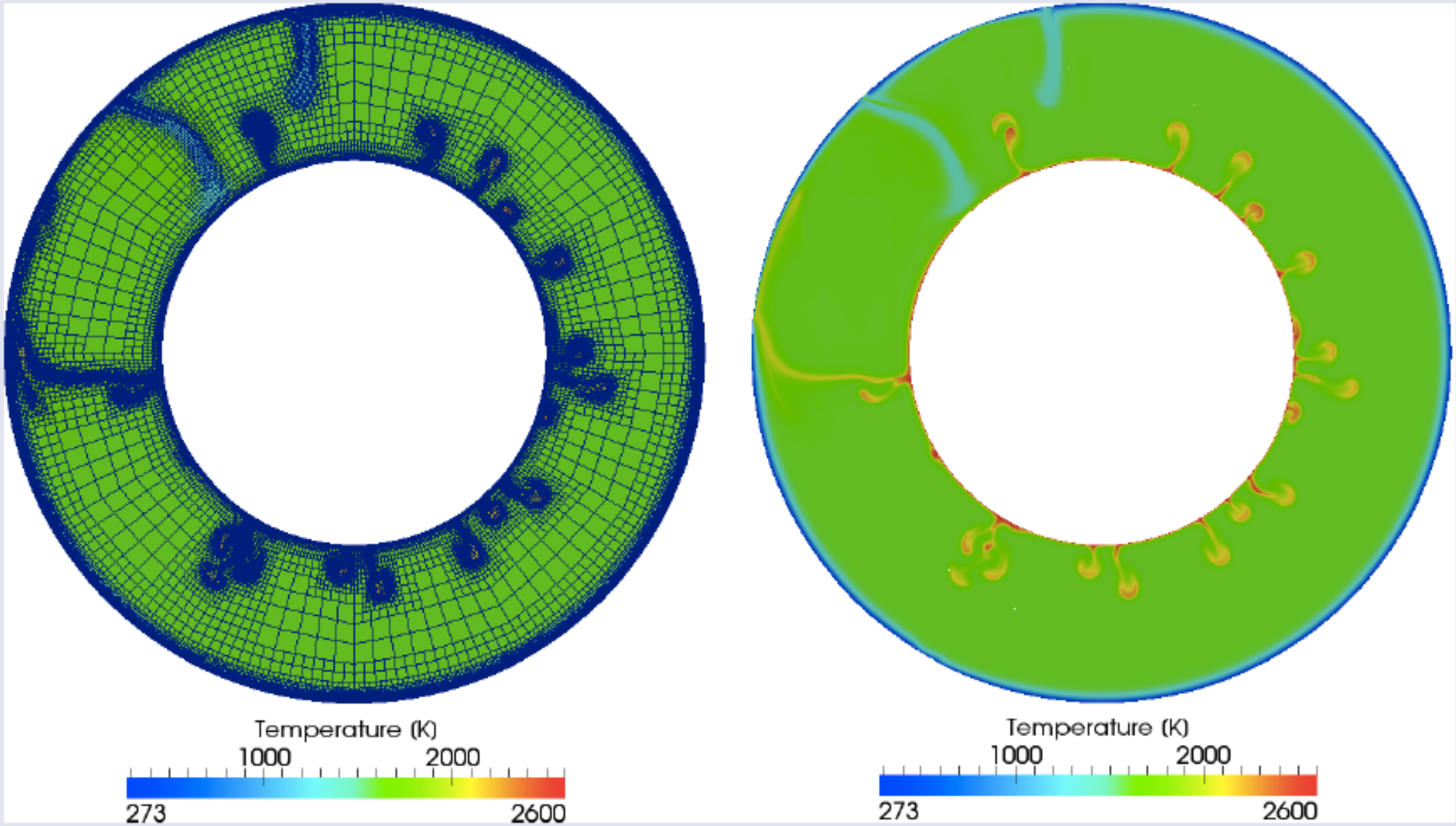
(sum up c_K in the cells with the largest/smallest error until you reach fraction *a* of the error)

Mark those cells for refinement/coarsening

Mesh refinement options

- Strategies: (nonadiabatic) temperature /pressure, composition, density, velocity, viscosity, thermal energy density…
- Refinement criteria scaling factors
- min/max refinement level function
  - Phase transitions / jump in material properties
- Additional refinement times
  - Onset of new processes (convection? melting? plate velocities?)

Mesh adaptation

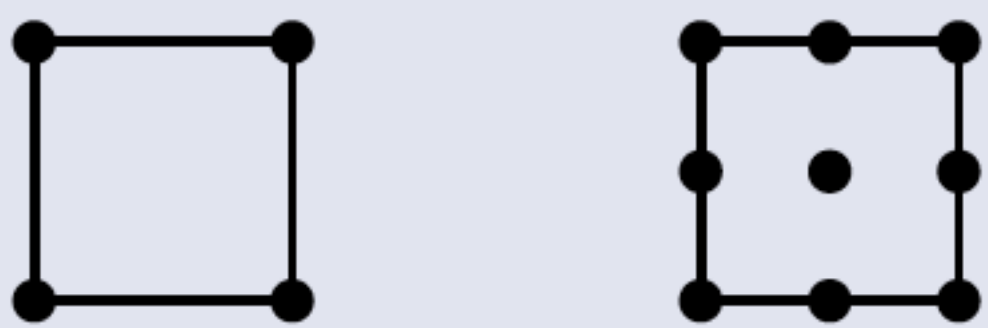


Discretization

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- Finite element method
- Uses Cartesian coordinates (mapping for curved boundaries)
- Free choice of finite element basis functions
  - Stability: choose polynomial degree of velocity one order higher than for pressure (e.g. linear and quadratic)

Pressure



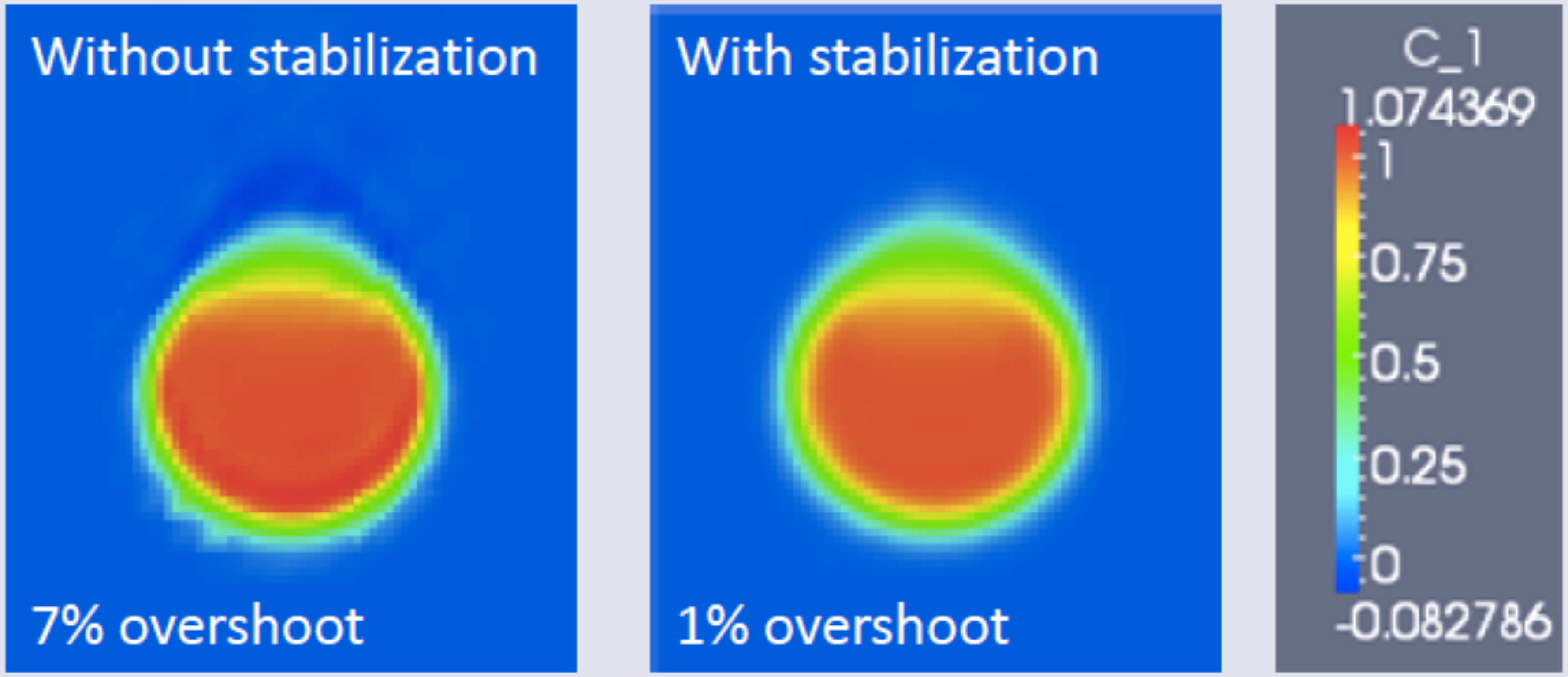
Velocity, temperature, composition

Discretization

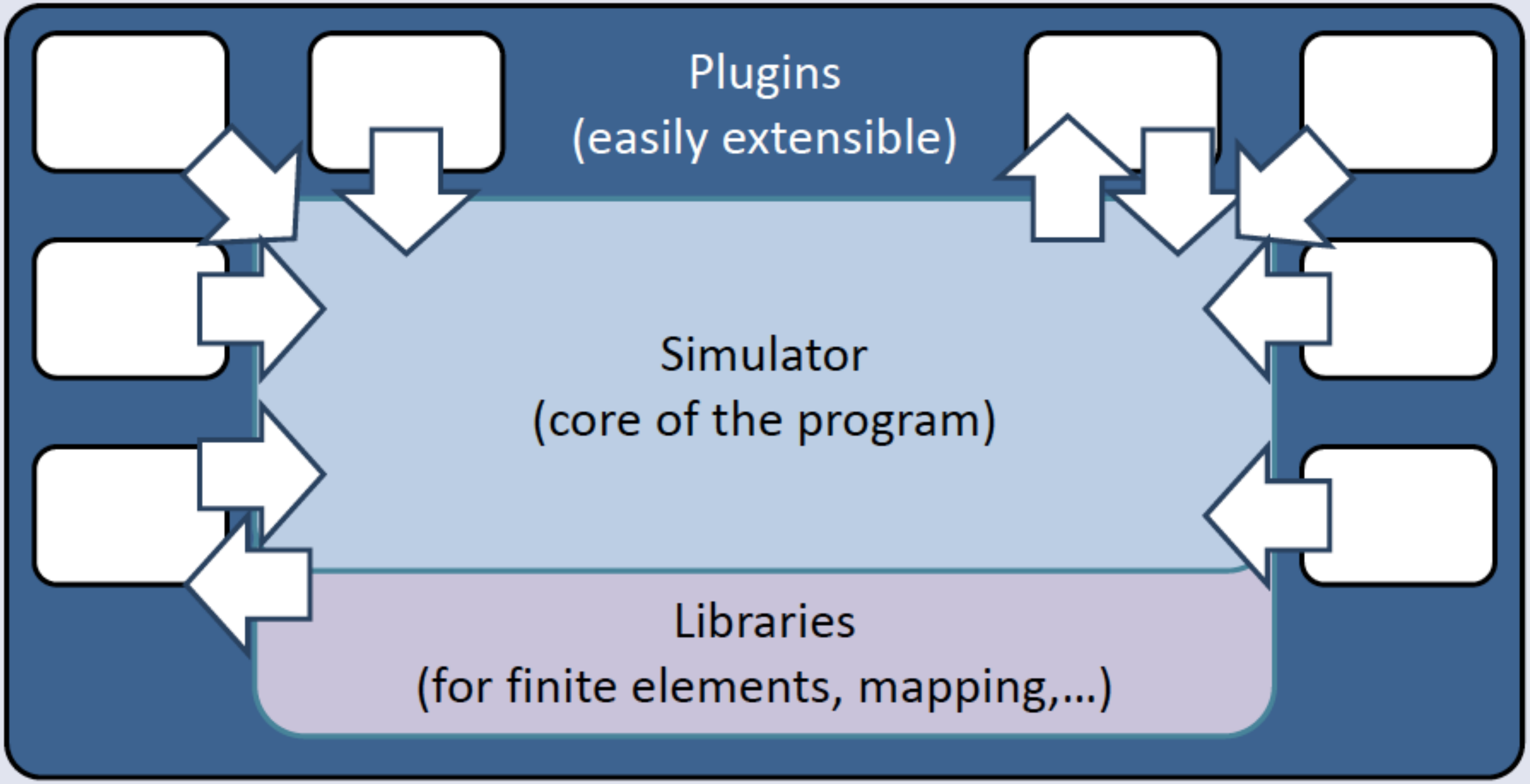
- Modified temperature/composition equation:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T - \nabla \cdot (\kappa + \nu_h(T))\nabla T = \gamma$$

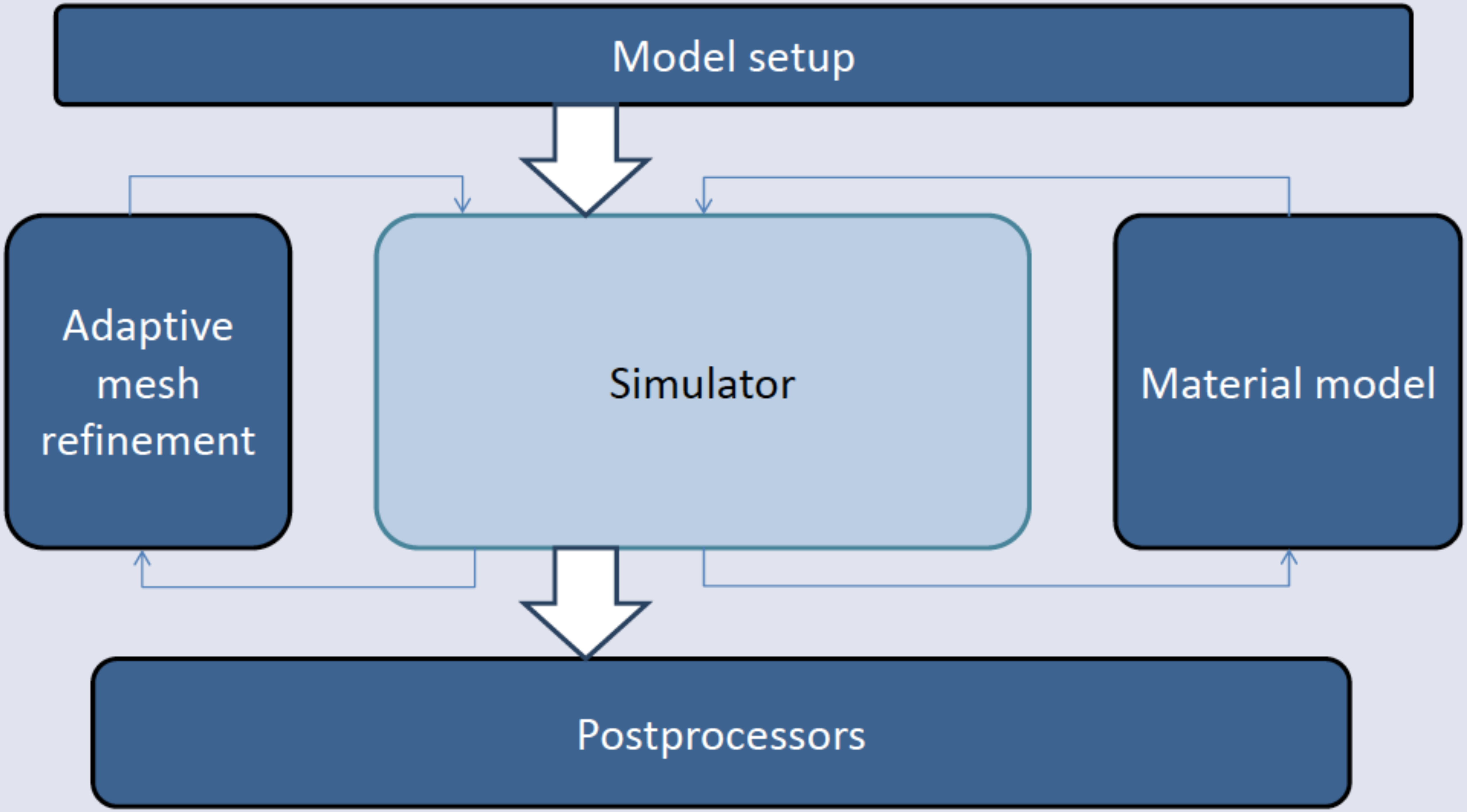
- Result:



Modularity


Plugins
(easily extensible)
Simulator
(core of the program)
Libraries
(for finite elements, mapping,...)

Modularity


Model setup
Adaptive mesh refinement
Simulator
Material model
Postprocessors

Modularity

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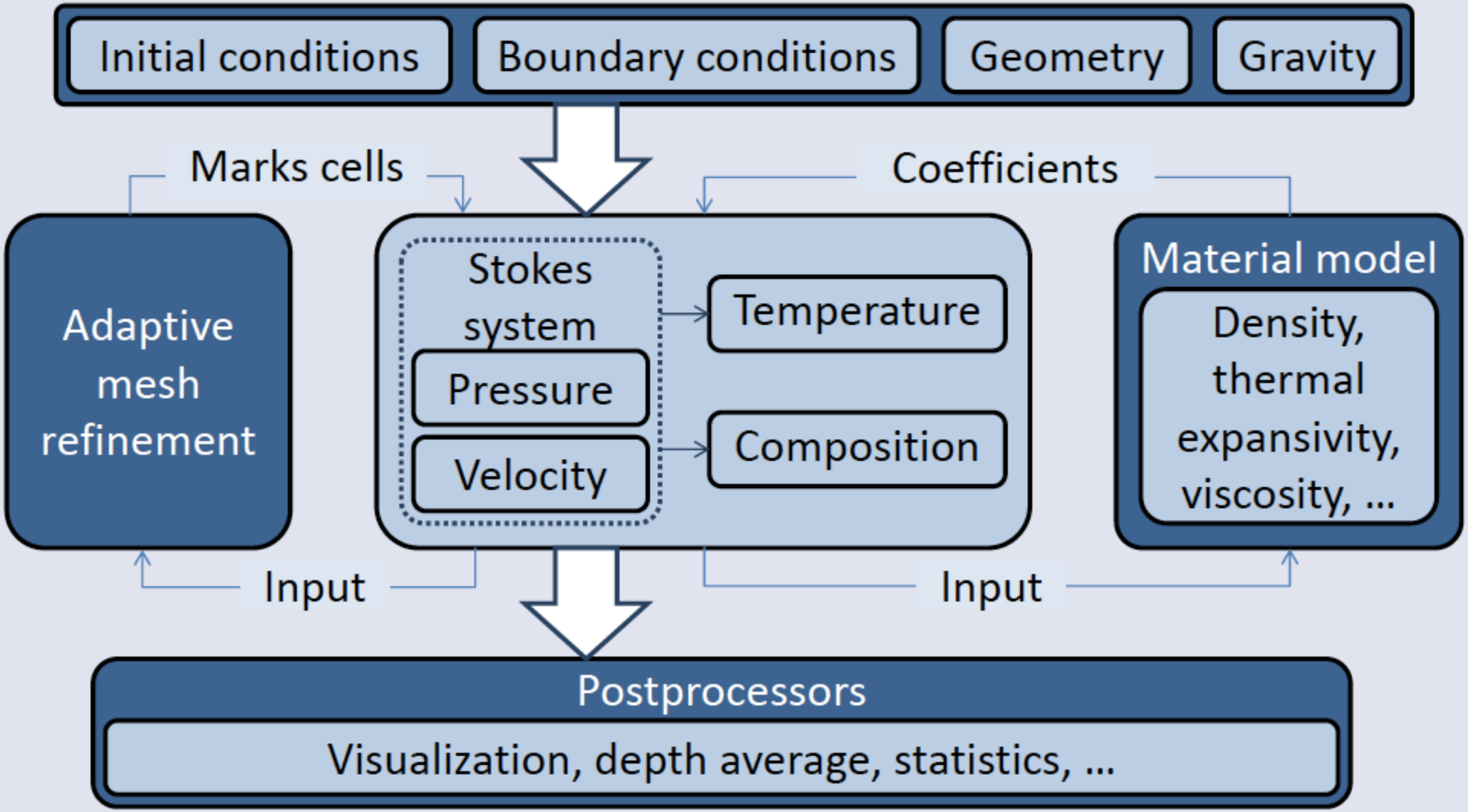

Checkpointing

- After crash of program
- Use the final state of one model as initial condition for a series of models

→ Restart required

- Aspect creates checkpoint files
- Possibility to change parameters in restarted model (material laws, postprocessors)

Building on libraries

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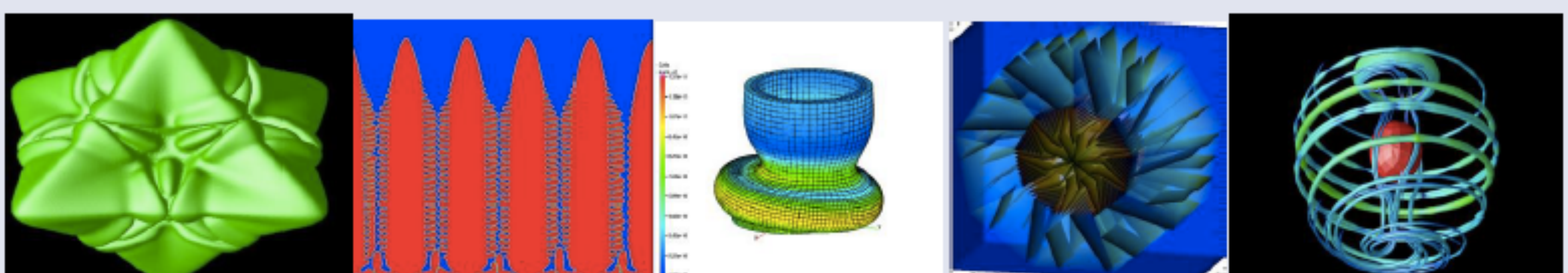
deal.II

- Meshes, finite elements, discretization: http://www.dealii.org/
- a C++ program library targeted at the computational solution of PDEs using adaptive finite elements



Efficient solvers

- Temperature: Conjugate gradient with preconditioner (LU decomposition)
- Stokes system (pressure & velocity): Generalized minimal residual method with preconditioner (includes conjugate gradient solves & algebraic multigrid)

Short term

- Melt transport ✓
- Active tracers ✓
- Approximations $\rightsquigarrow$ benchmarking efforts
- Robust nonlinear solvers
- Geoid
- Better experience for beginners (tutorials, installation, etc.)

Long term

We need to be bold!

- Sensitiviy analysis, inverse problems, uncertainty quantification?
- Surface processes
- Elastic rheology
- large scale, matrix-free, geometric multigrid
- Long-term tectonics
- and then take over whole geoscience cc

Part II
Discontinuous Galerkin method with a bound preserving limiter method for the Advection of non-Diffusive Fields in Solid Earth Geodynamics

Mathematical Modeling

$$-\nabla \cdot (2\eta(C)\epsilon(\mathbf{u})) + \nabla \mathbf{p} = \rho(C)\mathbf{g}, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{C} = 0, \tag{3}$$

$\mathbf{u}$, p and C are variables of velocity, pressure and composition

$\eta(C)$ viscosity and $\rho(C)$ density

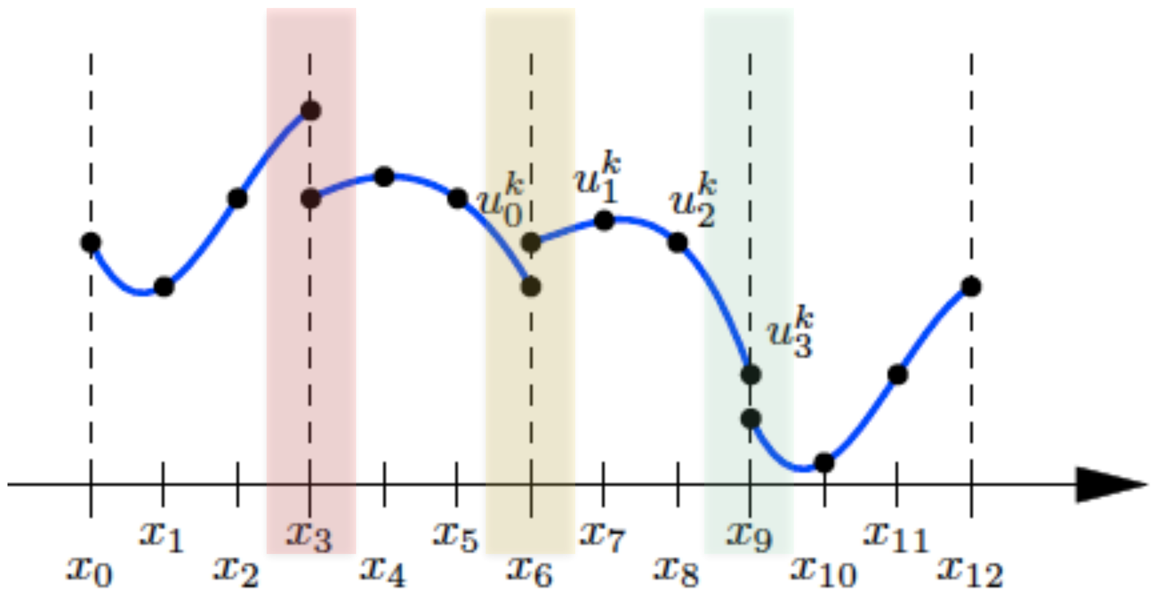
(1)+(2) Incompressible Stokes equation

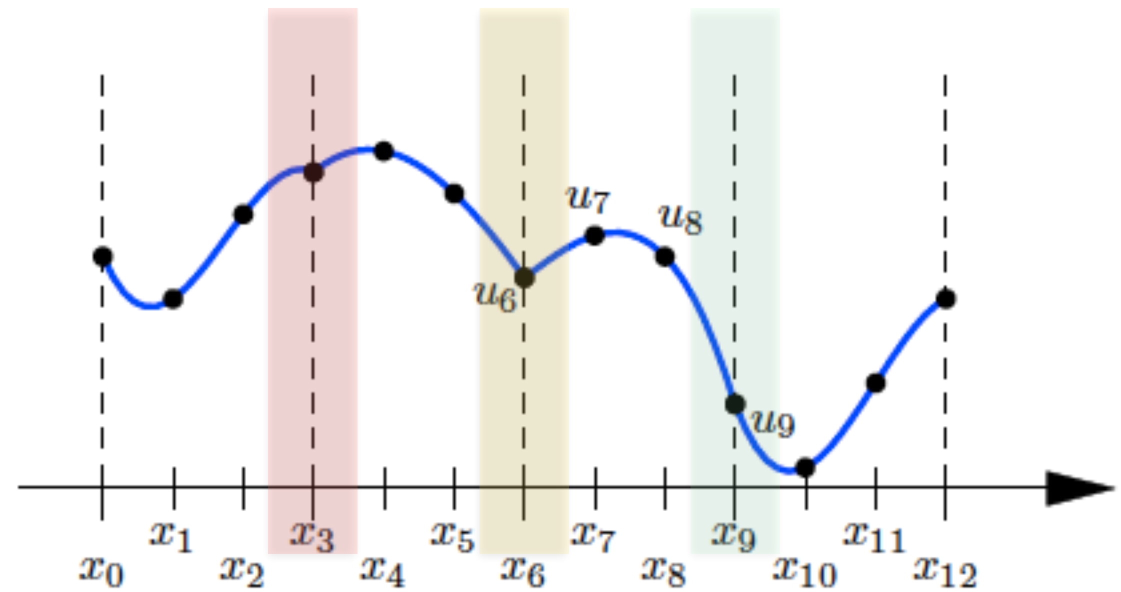
(3) advection/convection equation

The unique solution $C(x,t)$ satisfies $0 \leq C(x,t) \leq 1$ for any $0 \leq x \leq 1$ if given that the initial condition satisfies $0 \leq C_0(x) \leq 1$.

Overshoot $C(x,t) > 1$; Undershoot $C(x,t) < 0$;

DG-FEM v.s. CG-FEM





DG-FEM & CG-FEM

Galerkin approach: weak formulation

Element based piece-wise polynomial basis

Need to solve structured sparse matrix system

The DG-FEM solution is discontinuous between elements.

All operators of the DG-FEM are local.

The stability of DG-FEM is enforced through the flux choice.

<u>DG-FEM Double the number of degrees of freedom along the interfaces.</u>

Overshoot/Undershoot

DG-FEM: bound preserving limiter.

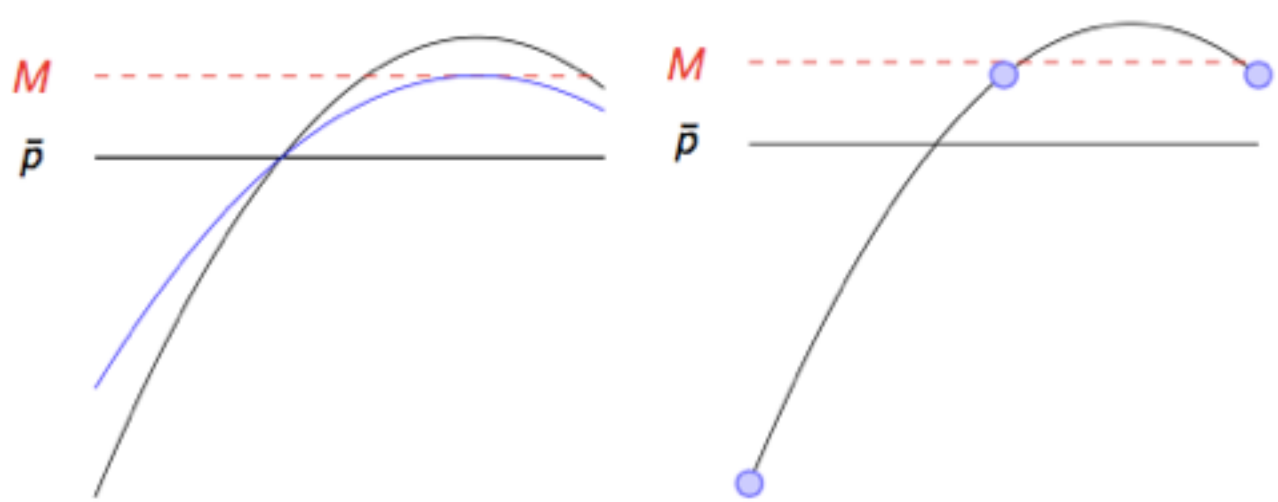
The limiter is a local post-processing procedure.

The framework is based on

Perthame and Shu, Numerische Mathematik, 1996: high order FV schemes with SSP Runge-Kutta can be written as a convex combination of several formal first order schemes.

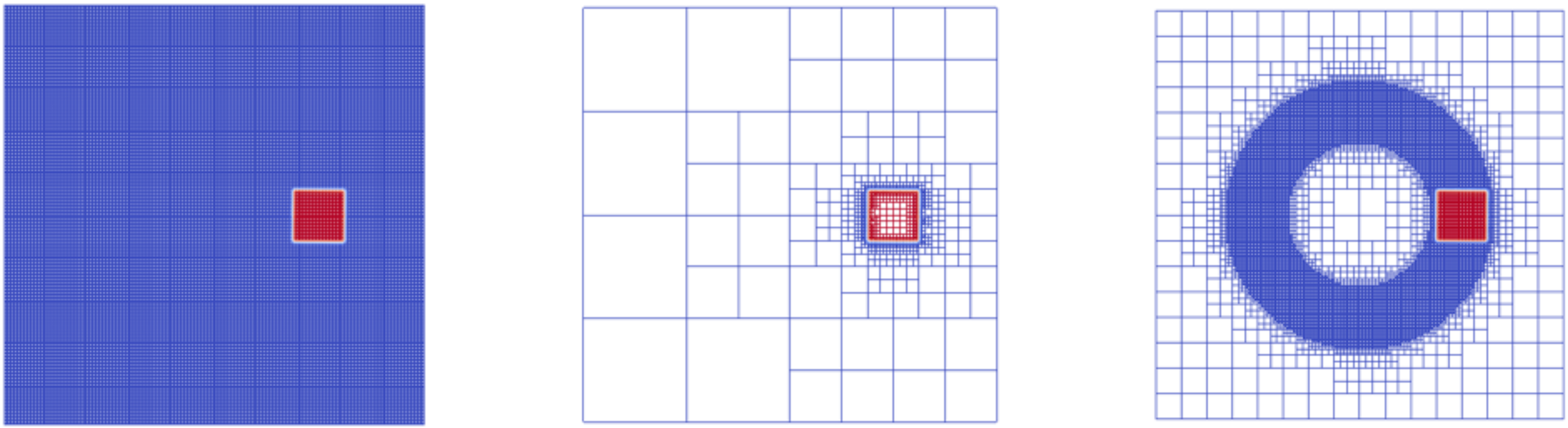
X.-D. Liu and S. Osher, SINUM, 1996: the simple scaling limiter.

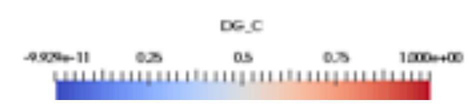
X.Z. and Shu, Journal of Computational Physics, 2010: the weak monotonicity.



Numerical experiments

Given a two dimentional steady flow with velocity field $\mathbf{u} = (-y, x)$

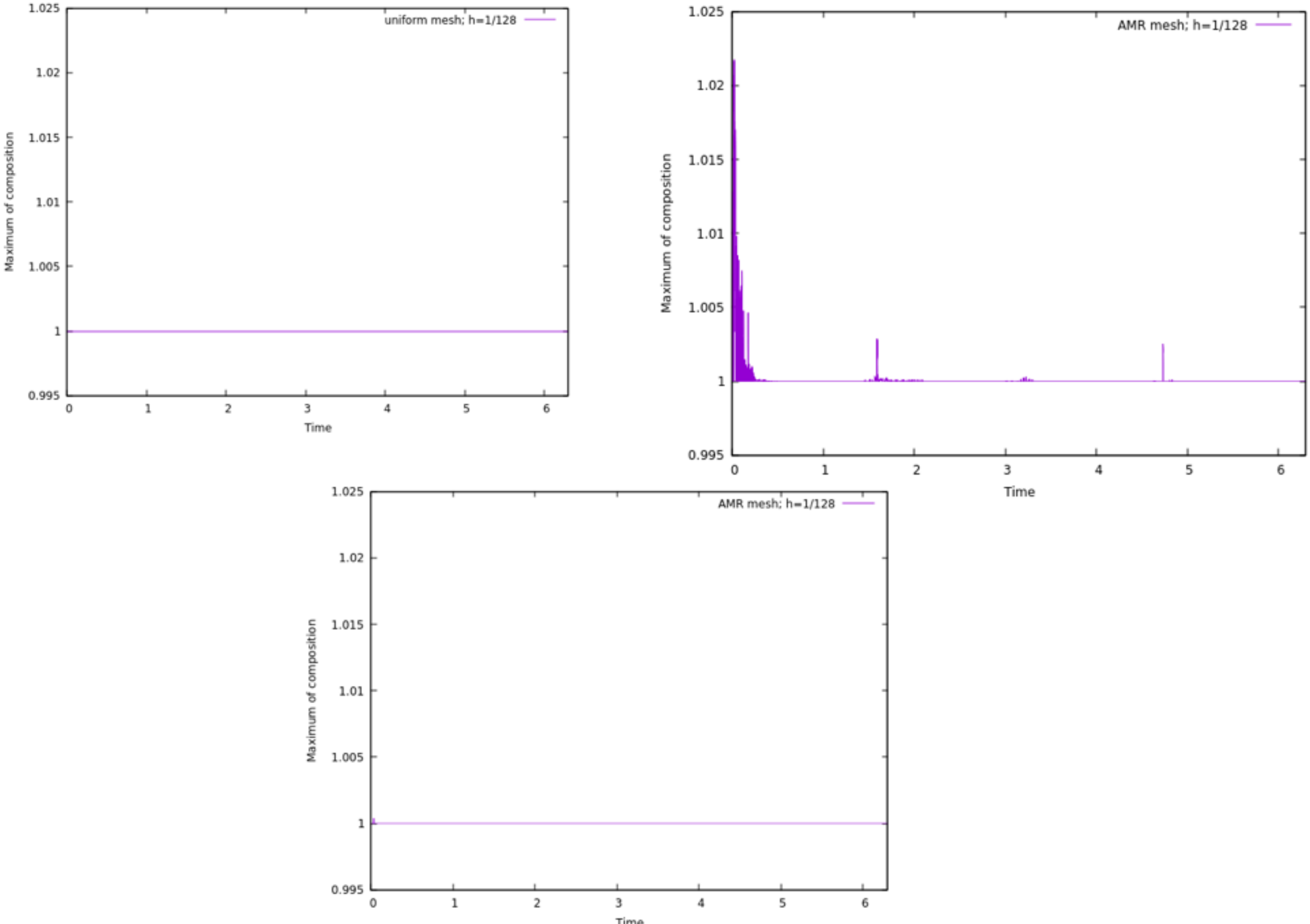




mesh size	# Cells	# Dofs(C)	Max	Min
Uniform Mesh				
1/128	65536	589824	1	-9.85052e-11
AMR with both refinement and coarsen				
1/128	1192	10728	1	-8.07723e-11
AMR with refinement only				
1/128	17554	157986	1	-9.46702e-11

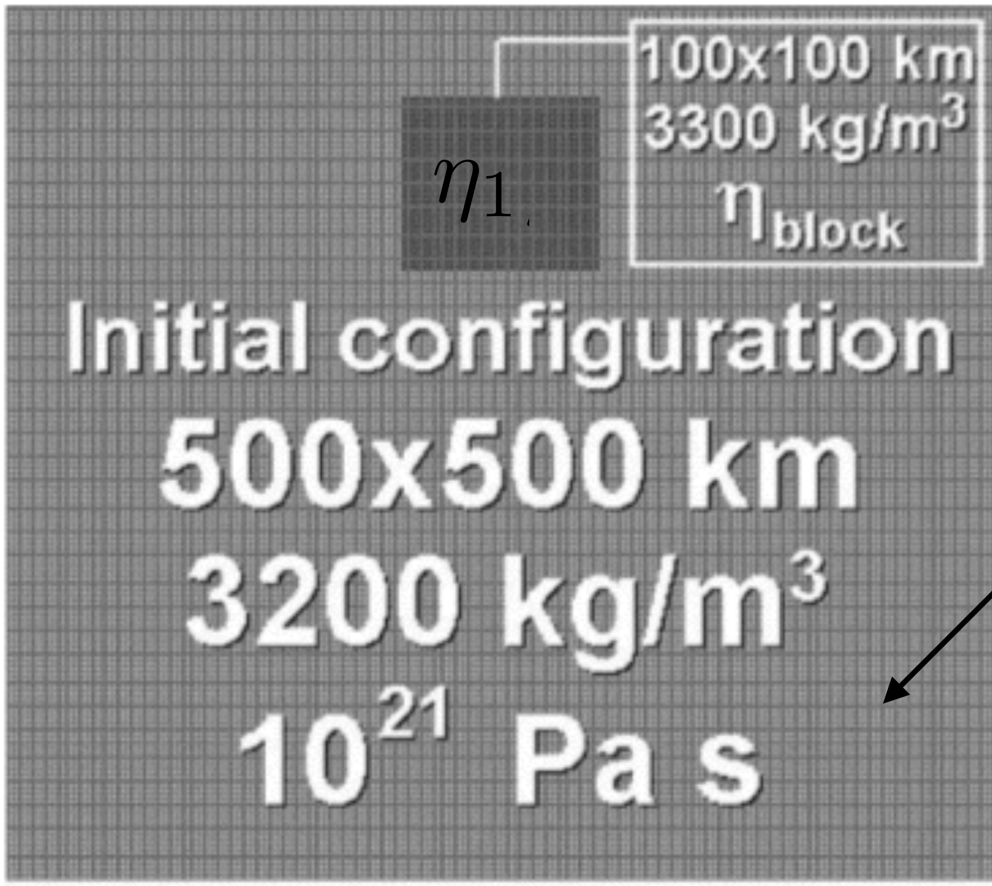
Table 1: Comparison of Numerical Test Results. Results are presented at time $6.283 \approx 2\pi$. For each viscosity ratio, we list the number cells resulting from the uniform mesh, AMR and AMR with refinement only, the number of degrees of freedom for the advection solver (C) and the overshoot/undershoot of the compositional field.

Numerical experiments



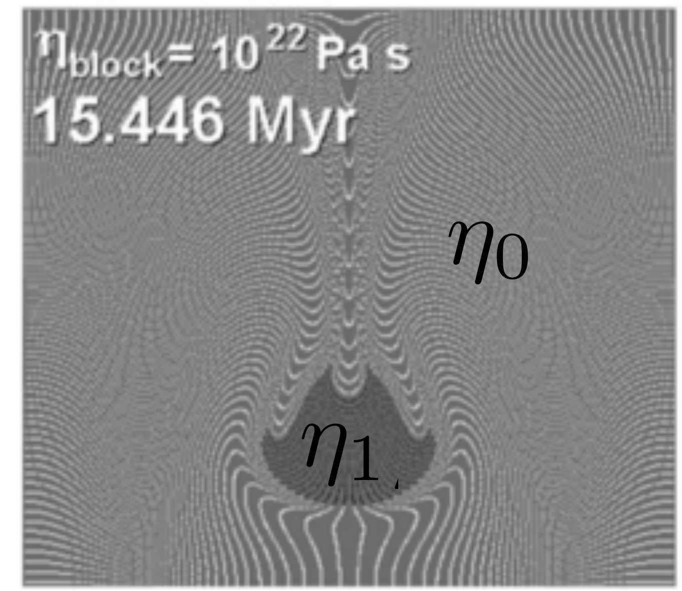
Test example: sinking hard box problem

T. V. Gerya, D. A. Yuen 2003

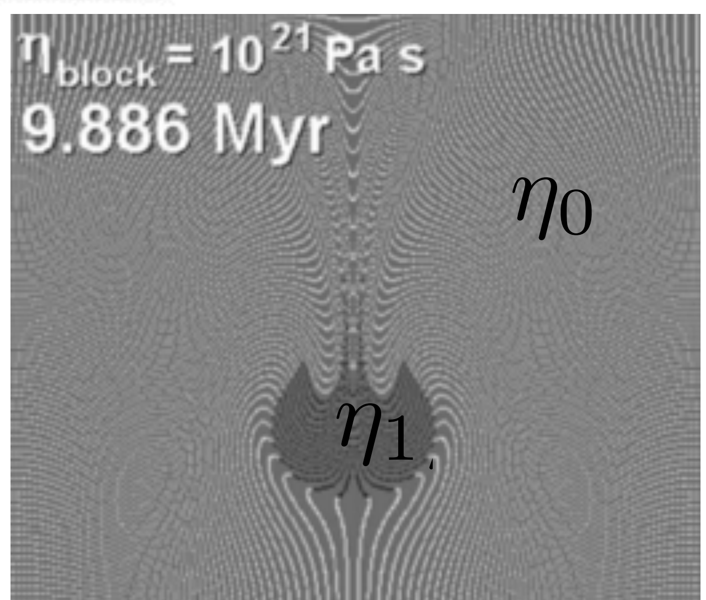


$$\eta_0 = 10^{21} Pa \cdot s$$

Markers' position only



$$\eta_1/\eta_0 = 10$$



$$\eta_1/\eta_0 = 1$$

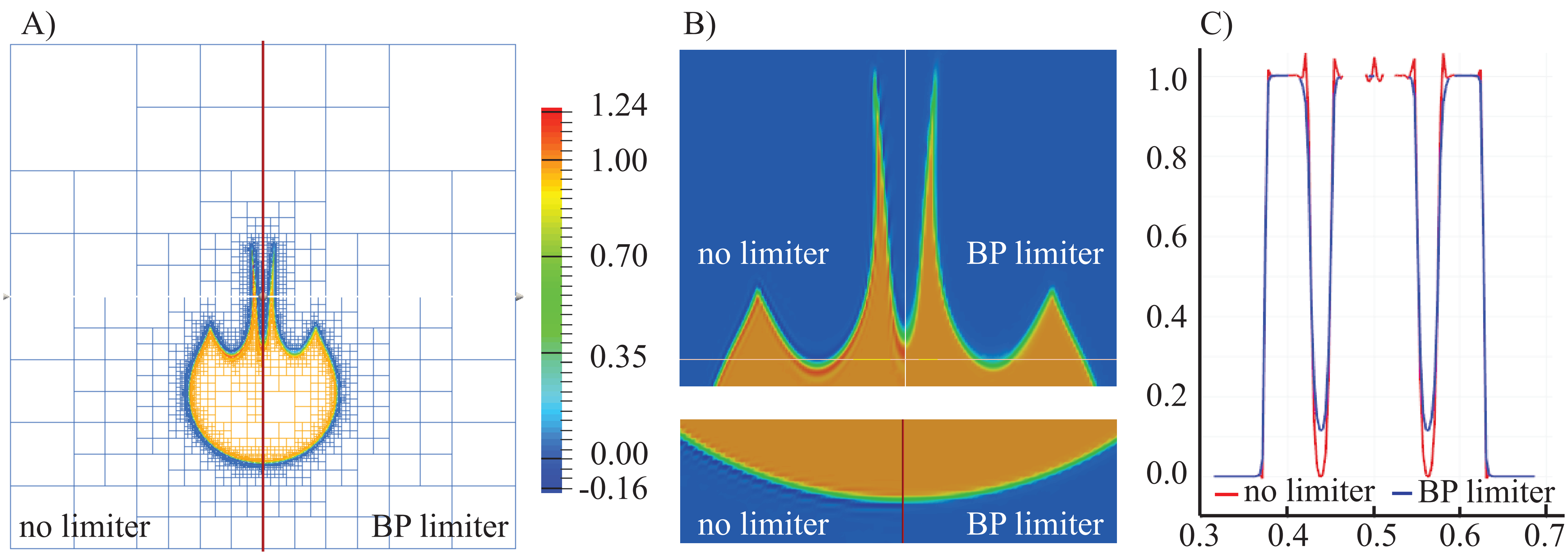
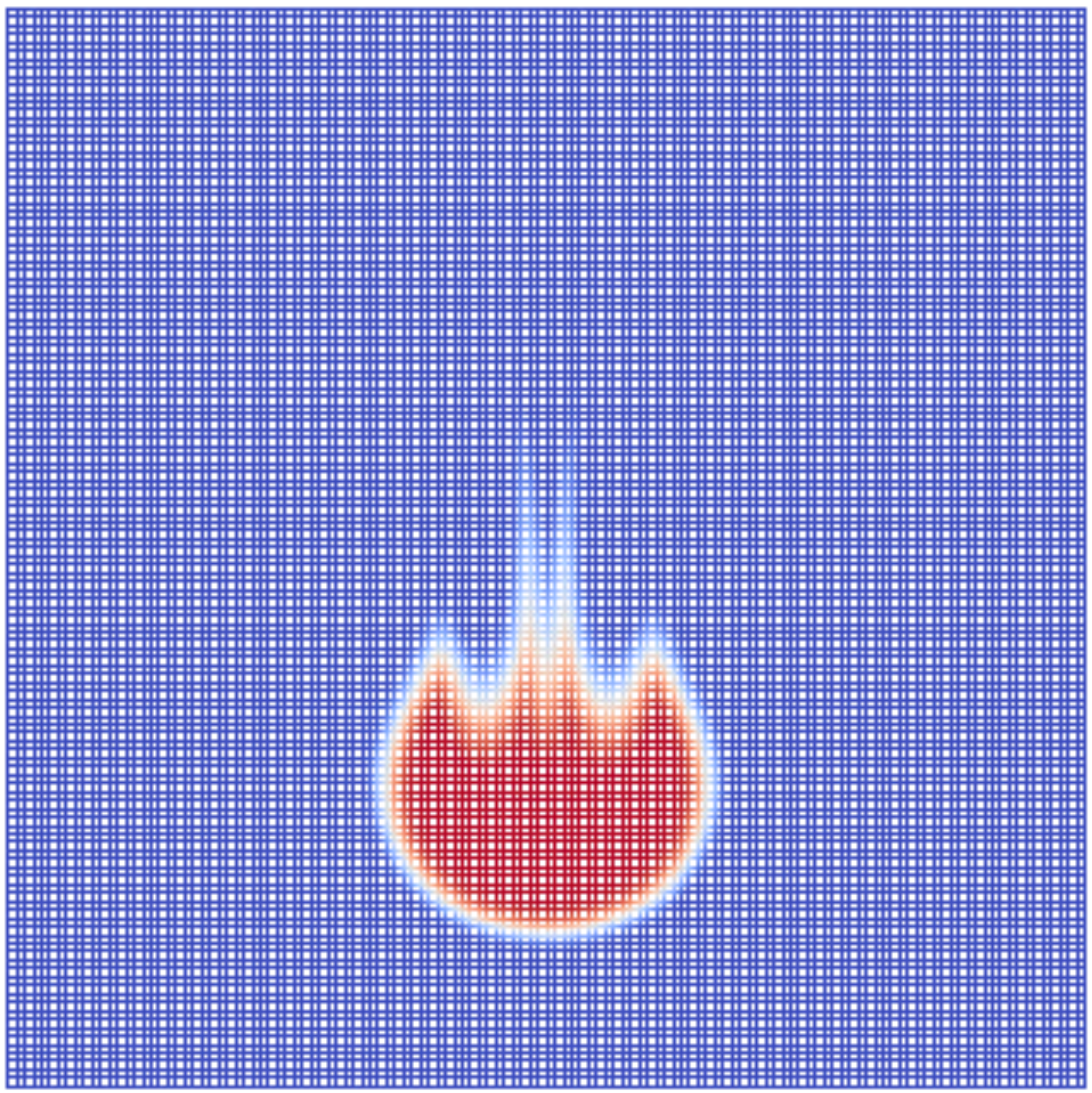
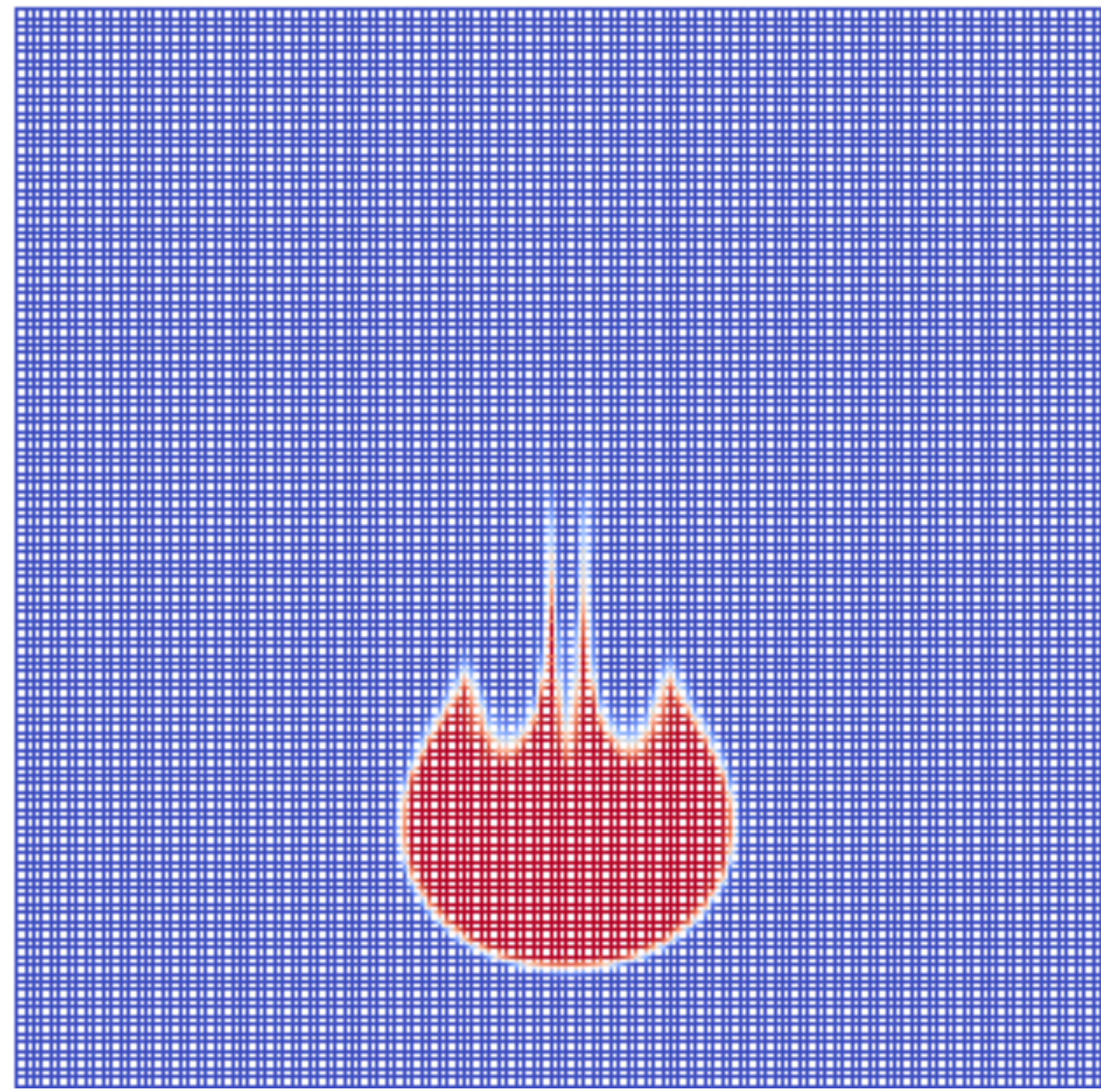


Figure 3: Comparison of DG with and without the BP limiter. A) Composition shown on AMR mesh at timestep 5000 for DG without limiter (left) and with limiter (right), B) Enlarged-view Comparison of Compositional Field for Top and Bottom of Falling Box, C) Horizontal profile across top. Location of profiles are shown in top sub-figure of (B).

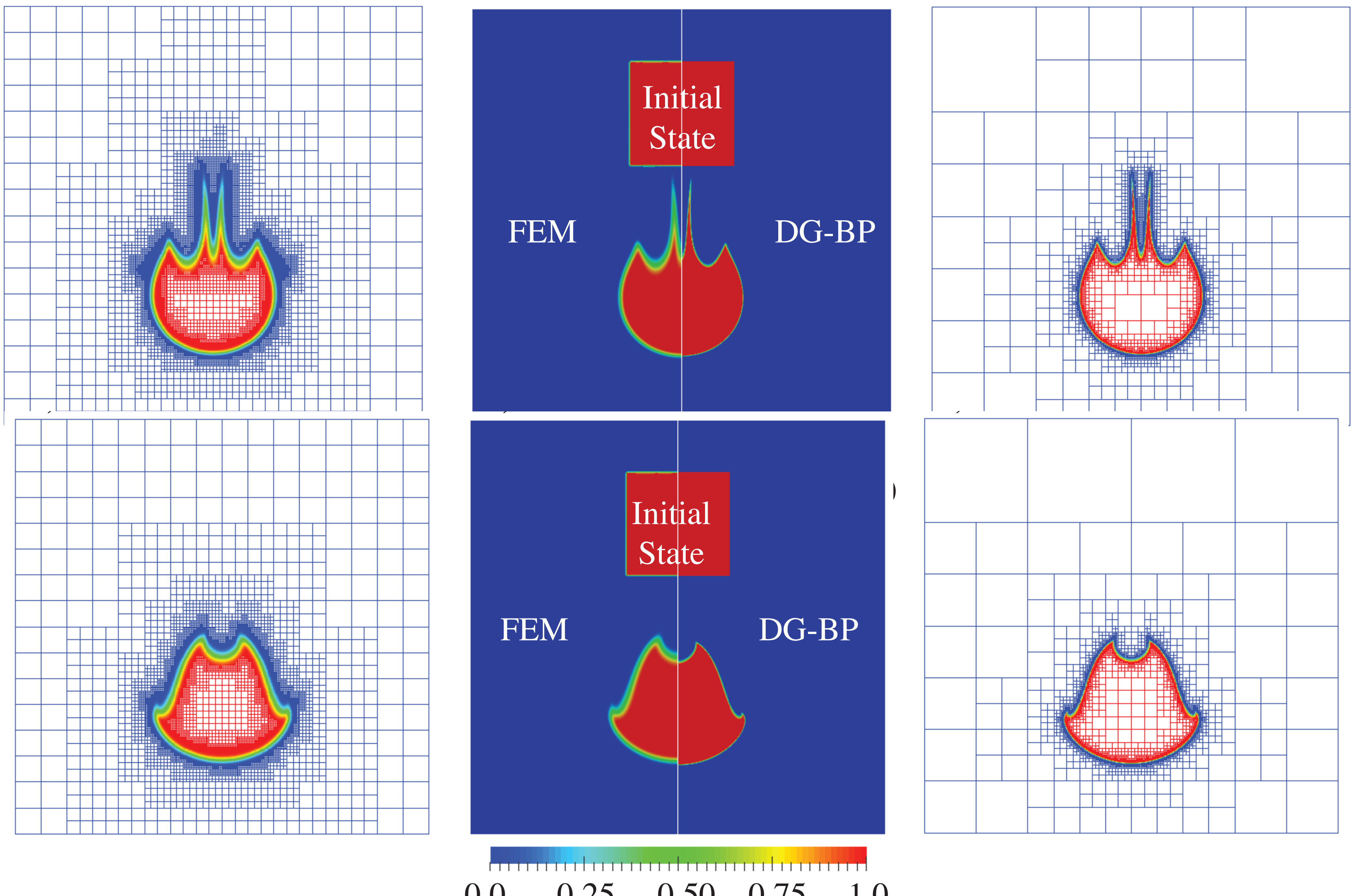
FEM (left) v.s. DGBP(right) uniform grid

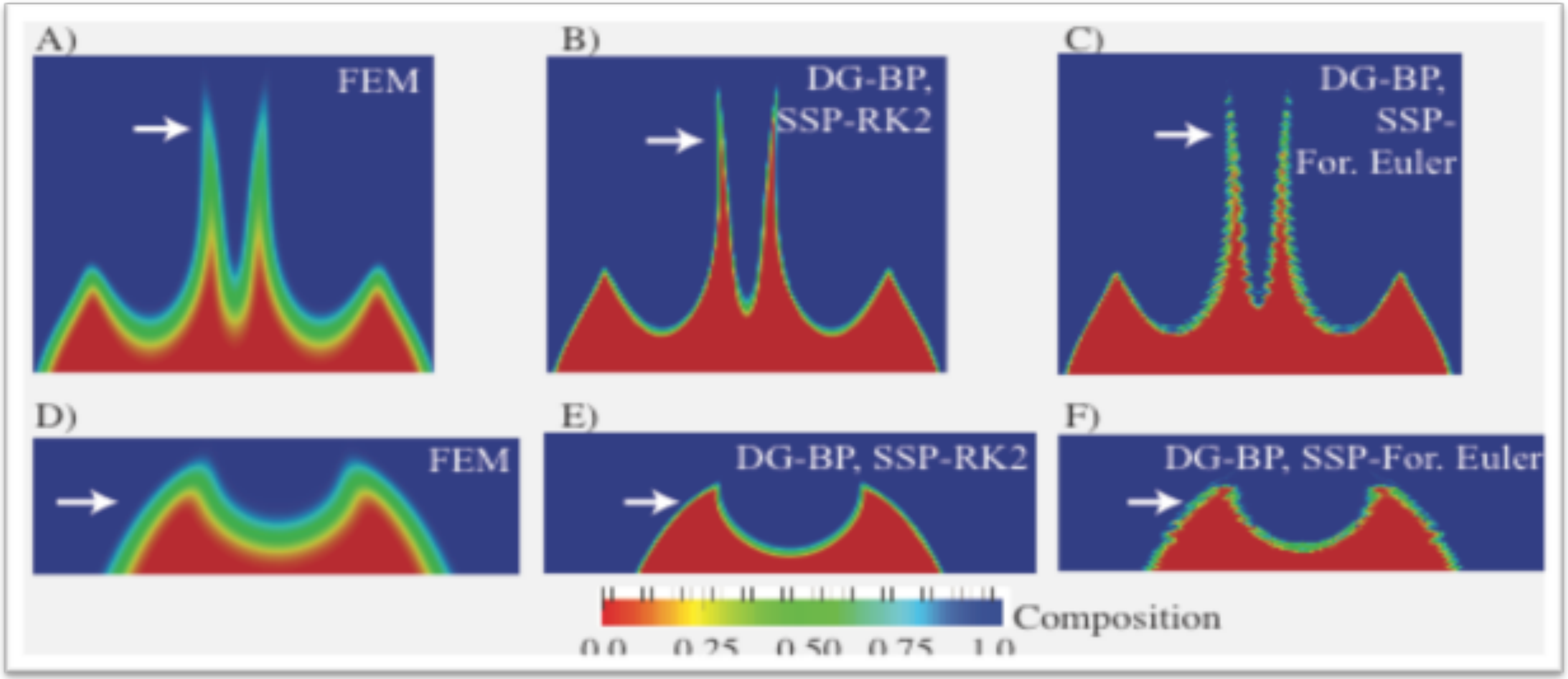


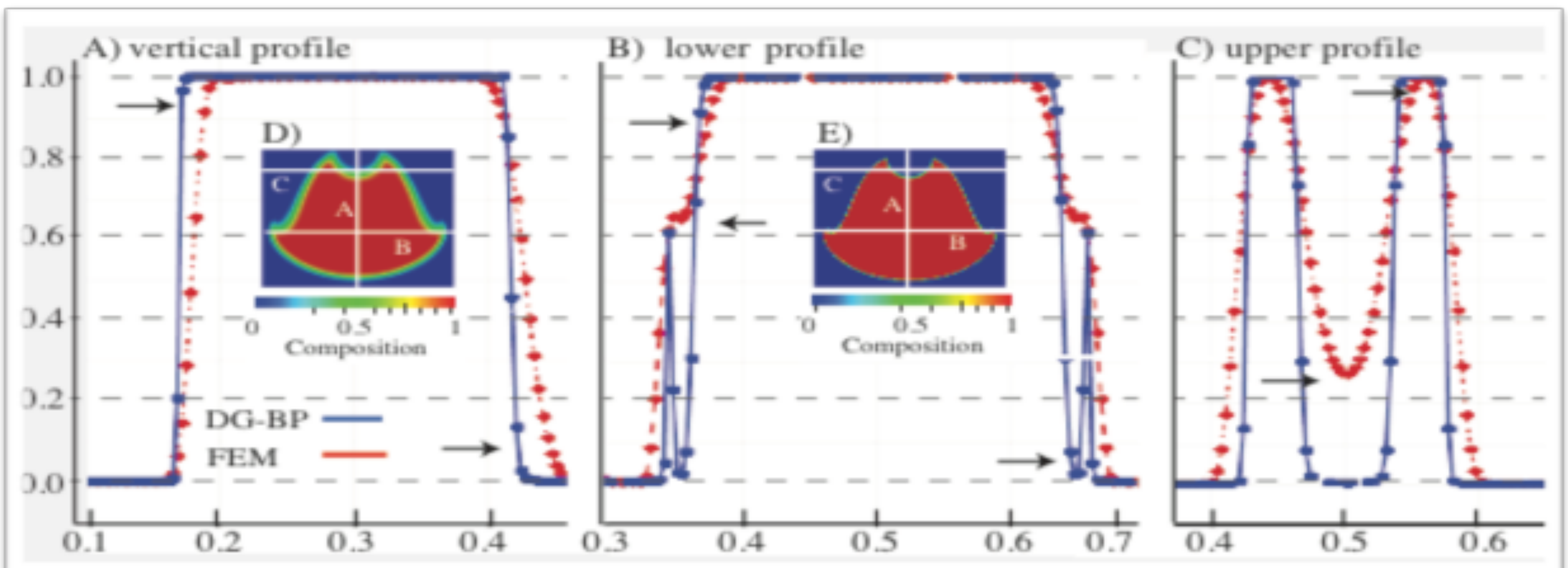


FEM v.s. DGBP AMR on

η_1/η_0	# Cells	# Dofs($\mathbf{u}+\mathbf{p}$, C)	Over (C, η)	Under (C, η)
FEM				
1	20404	(190543, 84677)	0.018%	0.100%
10	17020	(158827, 70581)	0.034%	0.072%
DG with BP Limiter, SSP RK2				
1	7759	(77384, 69831)	0.014%	0.022%
10	6271	(62628, 56439)	0.050%	0.015%




A)
FEM
B)
DG-BP, SSP-RK2
C)
DG-BP, SSP- For. Euler
D)
FEM
E)
DG-BP, SSP-RK2
F)
DG-BP, SSP-For. Euler
Composition
0.0 0.25 0.50 0.75 1.0


A) vertical profile
B) lower profile
C) upper profile
D)
E)
C
A
B
0 0.5 1
Composition
DG-BP
FEM
1.0 0.8 0.6 0.4 0.2 0.0
0.1 0.2 0.3 0.4
0.3 0.4 0.5 0.6 0.7
0.4 0.5 0.6

Conclusion

- Introduced ASPECT. Need more help? Subscribe ASPECT mailing list and ask questions.

- Developed a stable, accurate, and efficient method for compositional field advection equation: LDG+bound preserving limiter.

- Numerical results demonstrated that the proposed numerical method reduces the #cells and #DoFs significantly when AMR is used.

Thank you!