COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Tutorial III
Modelling Rayleigh-Taylor Instabilities

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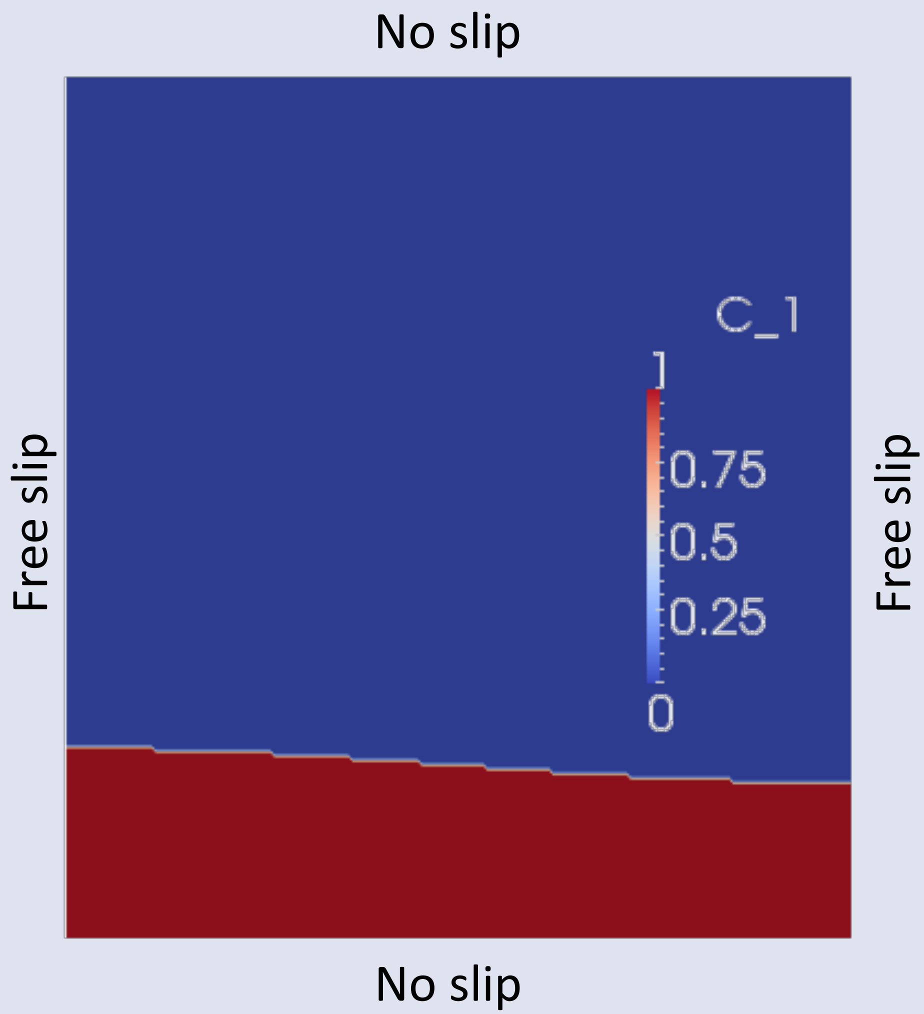
GeoMod2014

Overview

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- At the end of this tutorial, you should be able to:
  - Set up a model with compositional heterogeneities in Aspect
  - Use Aspect's function parser
  - Set up mesh independent initial conditions
  - Know a bit more about difficulties when reproducing benchmarks ☺

Setup: van Keken, 1997



- Geometry:
  Box: 0.9142 x 1
- Low-density layer at the bottom 20%, density difference: 1%
- Cosine initial perturbation to start upwelling

Tasks

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- We will split the class into multiple groups identified by the mesh refinement (number of global refinements)
- You will need to:
  1. modify the rayleigh_taylor.prm file to use your assigned refinement
  2. Run the simulation
  3. Visualize the results and make sure they are realistic
  4. report the first two peaks of root mean square velocity and their timing
  5. Note: to halt a simulation, press "Control-C"

Using ASPECT

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- We will begin by editing the input file

1. Change to the appropriate directory

    cd ~/ASPECT_TUTORIAL/models

2. Open the parameter file for editing

    gedit rayleigh_taylor.prm

Material model

```
subsection Material model
  set Model name = simple
  subsection Simple model
    set Viscosity                                         = 1e2
    set Thermal expansion coefficient                     = 0
    set Density differential for compositional field 1 = -10
  end
end
```

Initial conditions

Line 71:

```
subsection Compositional fields
  set Number of fields = 1
end

subsection Compositional initial conditions
  set Model name = function
  subsection Function
    set Variable names      =
    set Function constants  =
    set Function expression =
  end
end
```

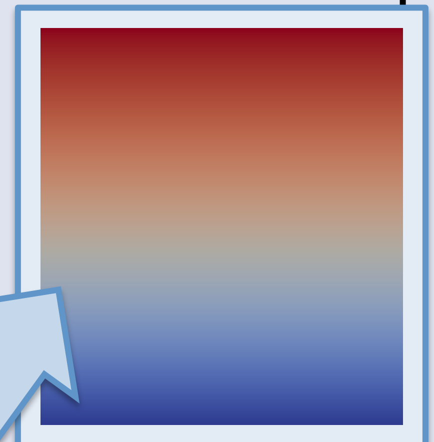
Initial conditions

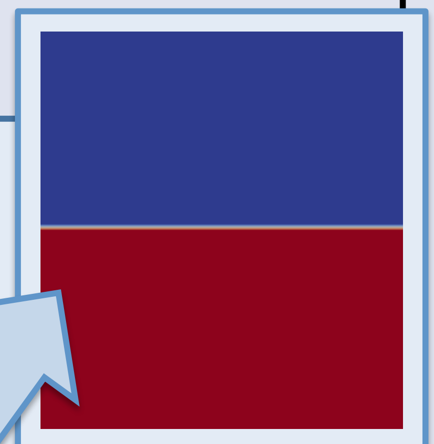
```
subsection Compositional fields
  set Number of fields = 1
end

subsection Compositional initial conditions
  set Model name = function
  subsection Function
    set Variable names      =
    set Function constants  =
    set Function expression =
  end
end
```

```
Example 1:
set Variable names            = x,z
set Function expression = sin(z)

Example 2:
set Variable names            = x,z
set Function expression = if(z > 0.5, 0, 1)
```





Initial conditions

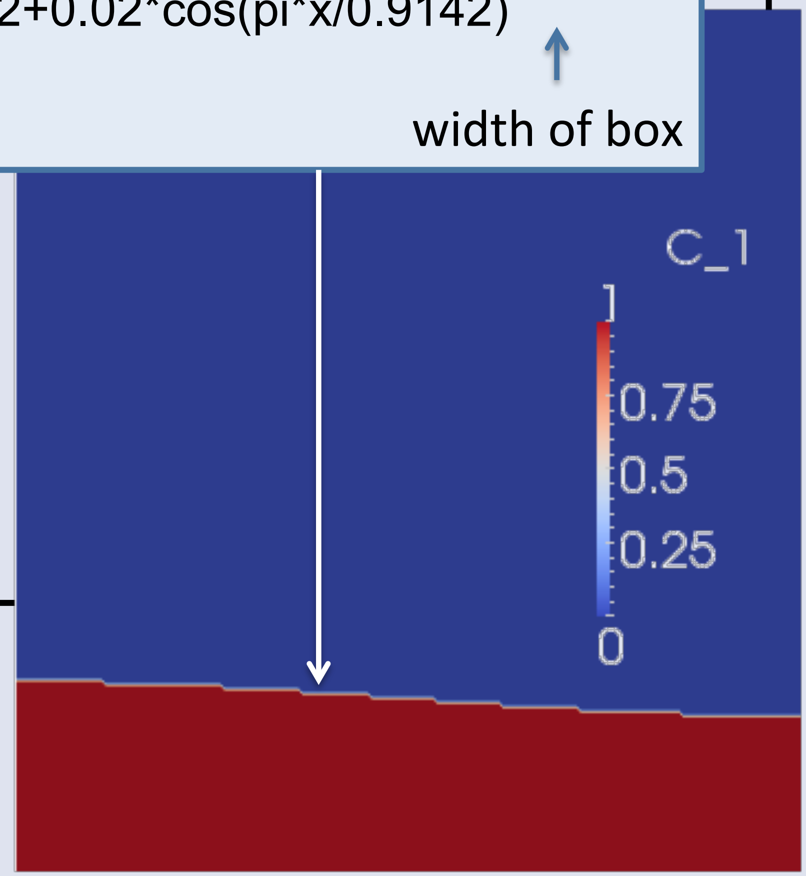
```
subsection Compositional fields
  set Number of fields = 1
end

subsection Compositional initial conditions
  set Model name = function
  subsection Function
    set Variable names      =
    set Function constants  =
    set Function expression =
  end
end
```

Interface:

0.2+0.02*cos(pi*x/0.9142)

width of box



Initial conditions

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
subsection Compositional fields
  set Number of fields = 1
end

subsection Compositional initial conditions
  set Model name = function
  subsection Function
    set Variable names      = x,z
    set Function constants  = pi=3.14159
    set Function expression =  if((z>0.2+0.02*cos(pi*x/0.9142)) , 0 , 1 )
  end
end
```

Variable names:
number of variables = dim (x,y)
OR
number of variables = dim+1
(x,y,t)

Syntax: *(else)*
if(condition, statement1, statment2)

```
if(condition)
   statement1;
else
   statment2;
```

Boundary conditions

```
subsection Model settings
  set Include adiabatic heating              = false
  set Include shear heating                  = false
  set Tangential velocity boundary indicators = 0,1
                                   # left and right
  set Zero velocity boundary indicators      = 2,3
                                   # bottom and top
end
```

Resolution

```
subsection Mesh refinement
  set Initial adaptive refinement        = 0
  set Initial global refinement          = 7
  set Time steps between mesh refinement = 0
end
```

This is what we want to change:

- Group 1: 5
- Group 2: 6
- Group 3: 7
- Group 4: 8

Running the model

aspect rayleigh_taylor.prm

Or in parallel

mpirun –np 2 aspect rayleigh_taylor.prm

The function parser

…in other modules:

- Initial temperature
- Boundary conditions (velocity & temperature)
- Heating model (radiogenic heating)
  - ➢ Crust / lithosphere / mantle
- Mesh refinement (min/max refinement level)
  - ➢ Phase transitions / jump in material properties
- Gravity model
  - ➢ Moon? Mars?

Heating model

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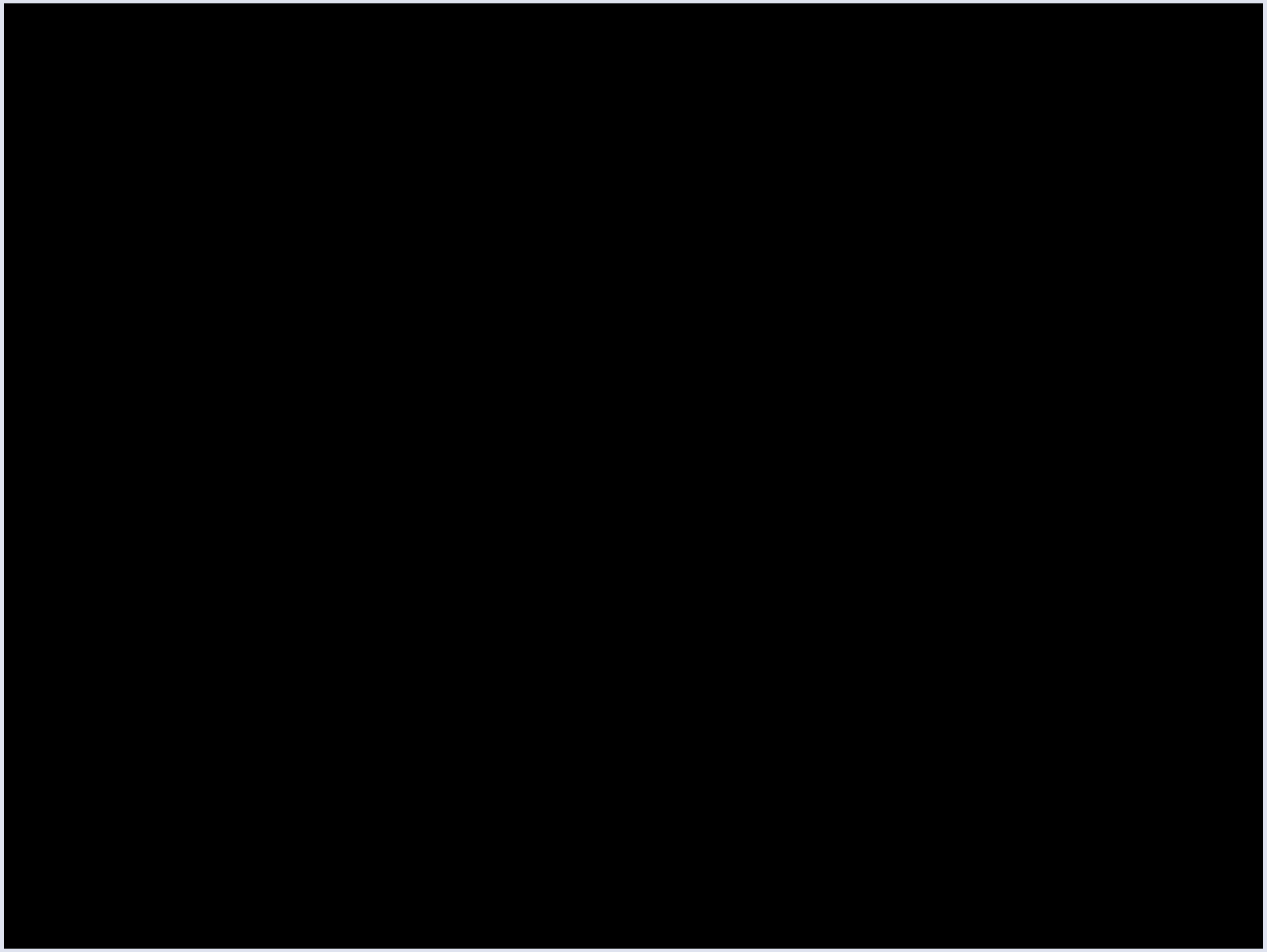


Visualizing results

1. With Paraview

    paraview

2. With Gnuplot

    cd rayleigh-taylor
    gnuplot
    plot "statistics" using 2:14 with lines

    time　　　vrms velocity

3. What are the times and velocity values of the first two peaks in root mean square velocity?

Visualizing results

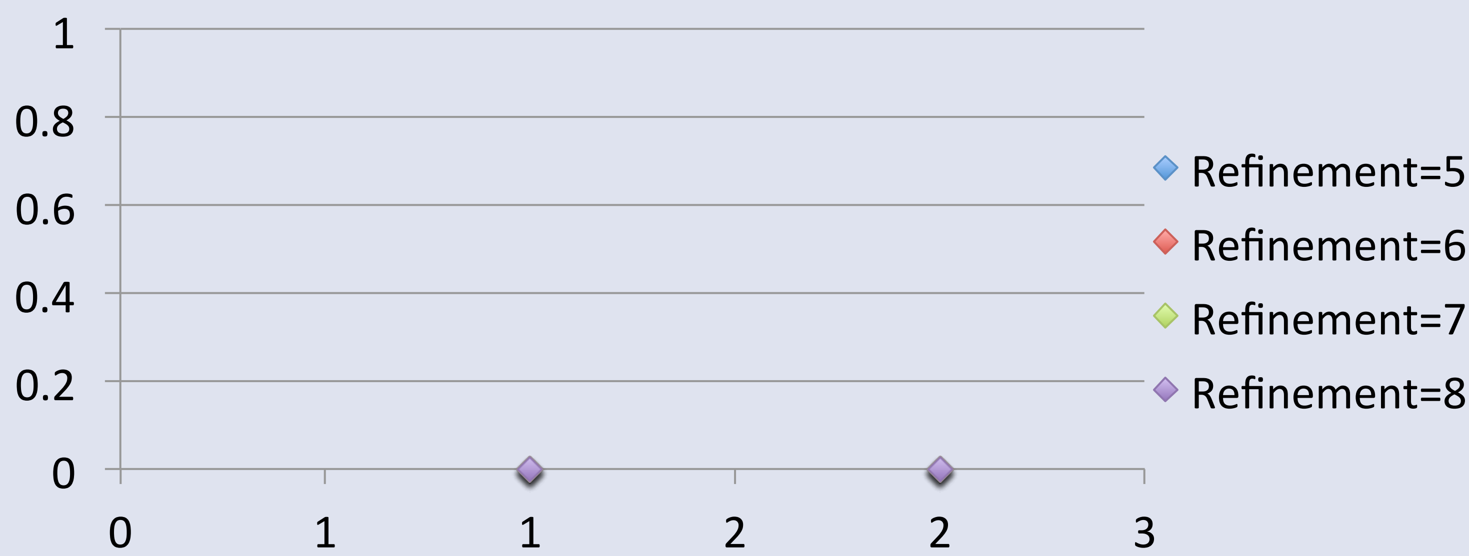
Header of the „statistics“ file:

1: Time step number
2: Time (seconds)
3: Number of mesh cells
4: Number of Stokes degrees of freedom
5: Number of temperature degrees of freedom
6: Number of degrees of freedom for all compositions
7: Iterations for temperature solver
8: Iterations for composition solver 1
9: Iterations for Stokes solver
10: Velocity iterations in Stokes preconditioner
11: Schur complement iterations in Stokes preconditioner
12: Time step size (seconds)
13: Visualization file name
14: RMS velocity (m/s)
15: Max. velocity (m/s)
16: Minimal value for composition C_1
17: Maximal value for composition C_1
18: Global mass for composition C_1

Results

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

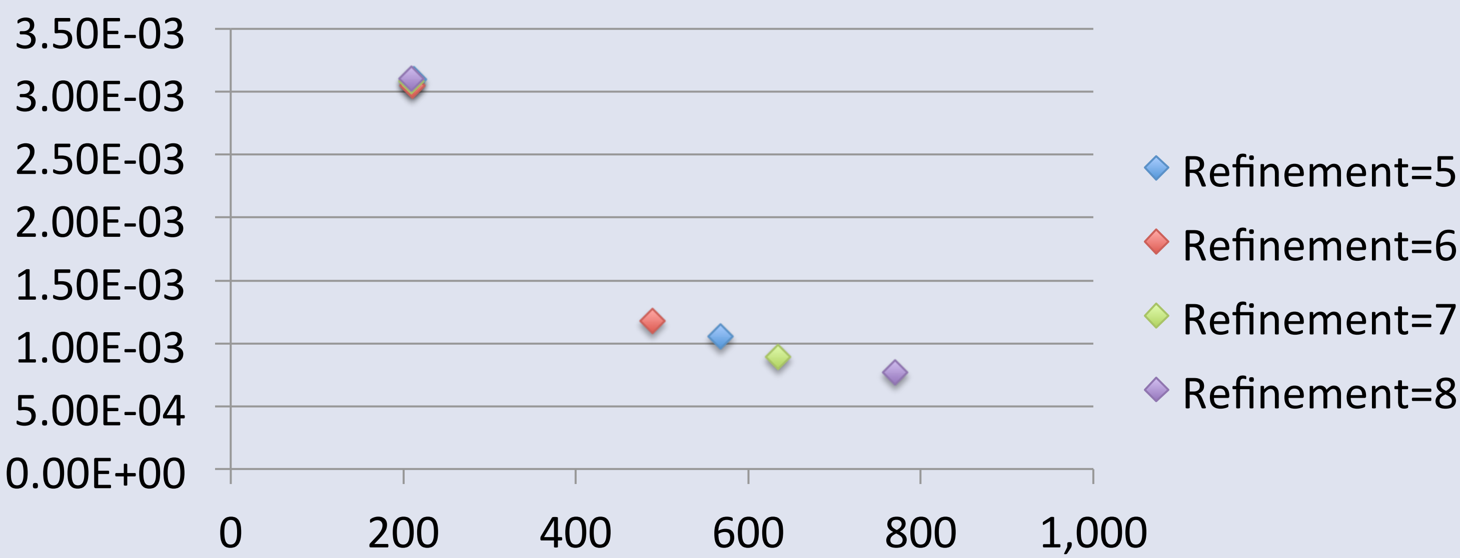
	Refinement=5	Refinement=6	Refinement=7	Refinement=8
1st peak (time)	(???)	(???)	(???)	(???)
1st peak (v_{rms})	(???)	(???)	(???)	(???)
2nd peak (time)	(???)	(???)	(???)	(???)
2nd peak (v_{rms})	(???)	(???)	(???)	(???)



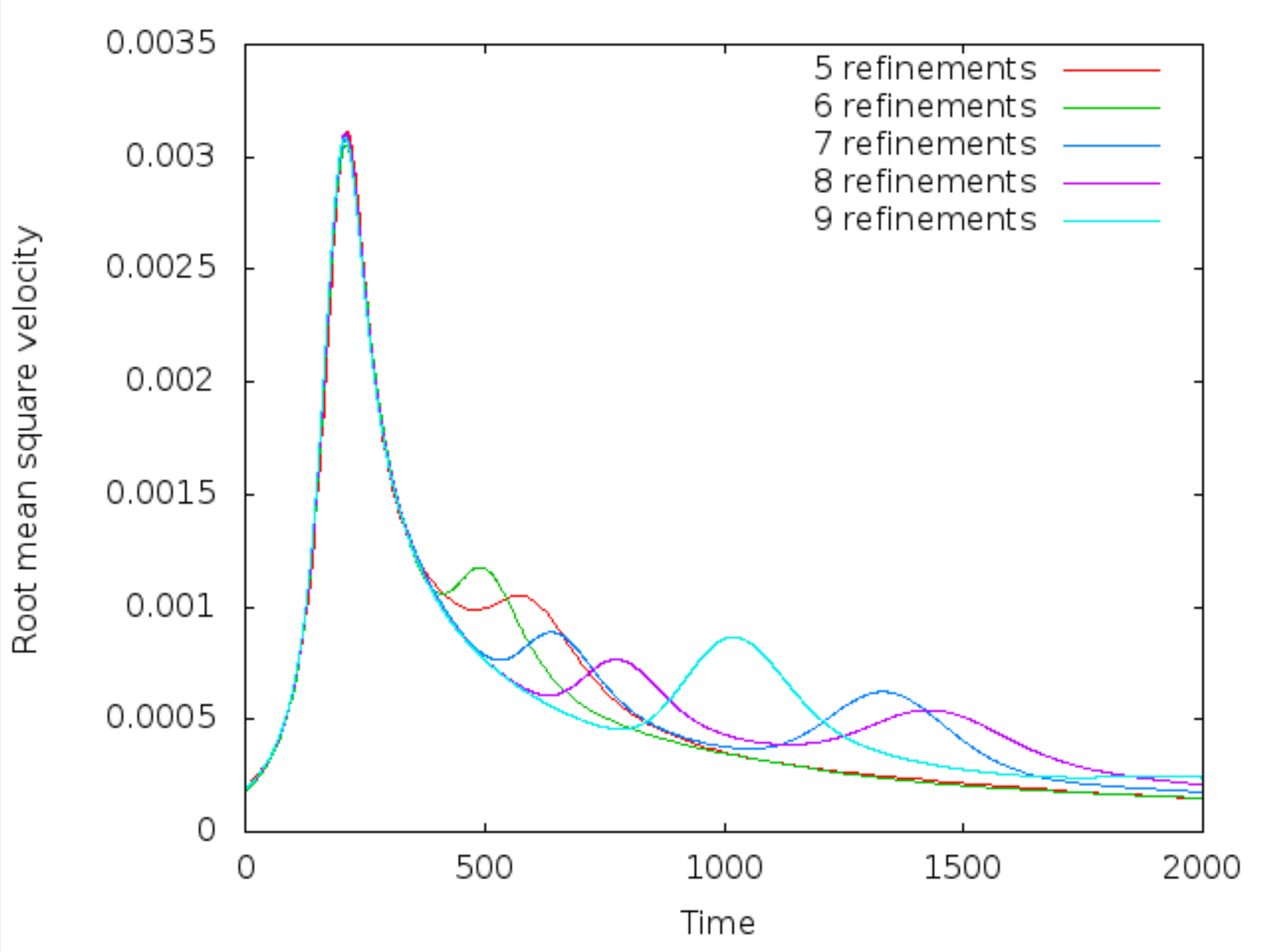
Backup slide with results

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

	Refinement=5	Refinement=6	Refinement=7	Refinement=8
1st peak (time)	2.1254e2	2.1017e2	2.0950e2	2.0954e2
1st peak (v_{rms})	3.1015e-3	3.0529e-3	3.0826e-3	3.1052e-3
2nd peak (time)	5.679e2	4.8927e2	6.3469e2	7.7013e2
2nd peak (v_{rms})	1.0509e-3	1.1751e-3	8.9403e-4	7.7073e-4

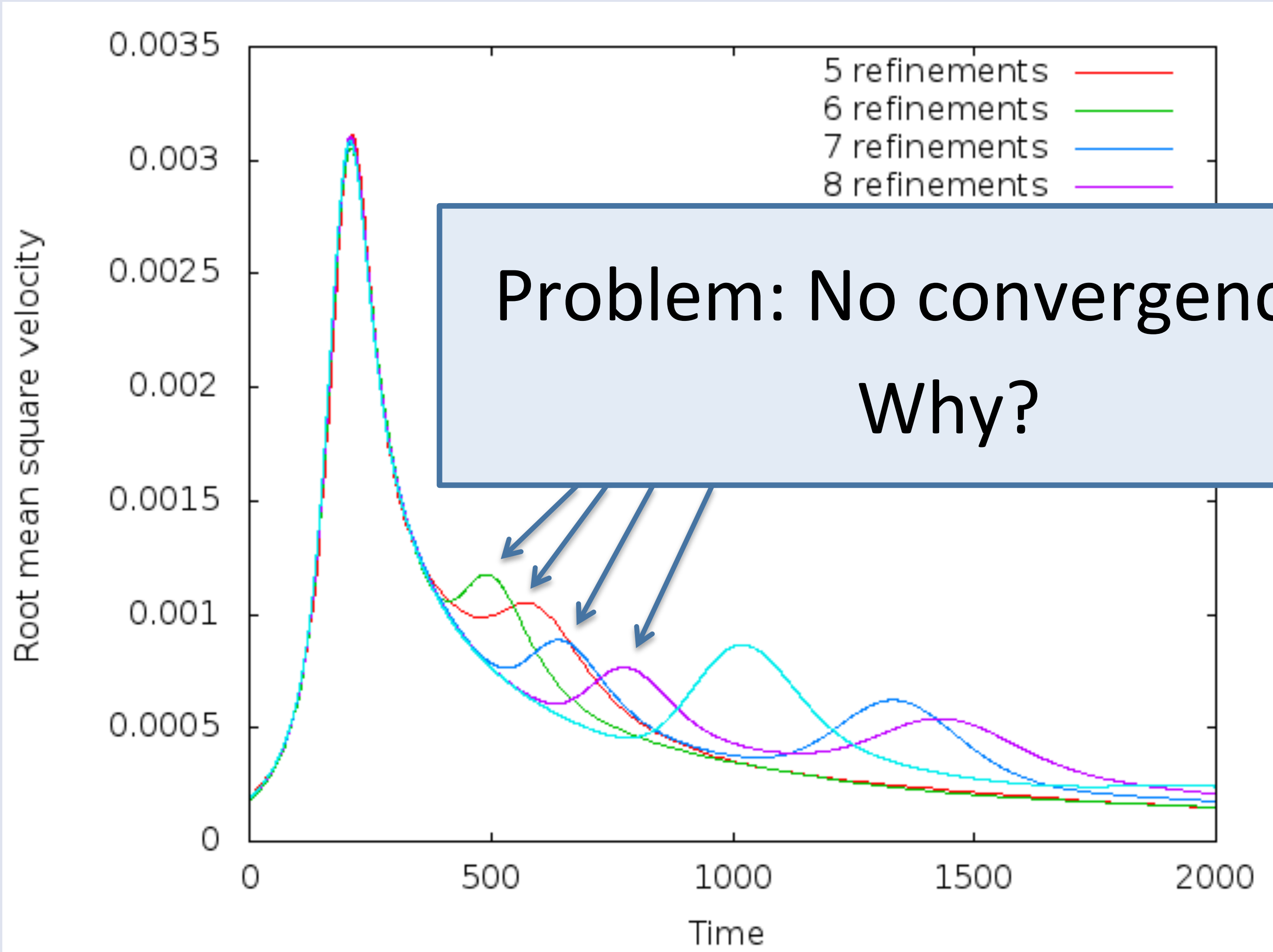


Results



Root mean square velocity
0.0035
0.003
0.0025
0.002
0.0015
0.001
0.0005
0
0
500
1000
1500
2000
Time
5 refinements
6 refinements
7 refinements
8 refinements
9 refinements

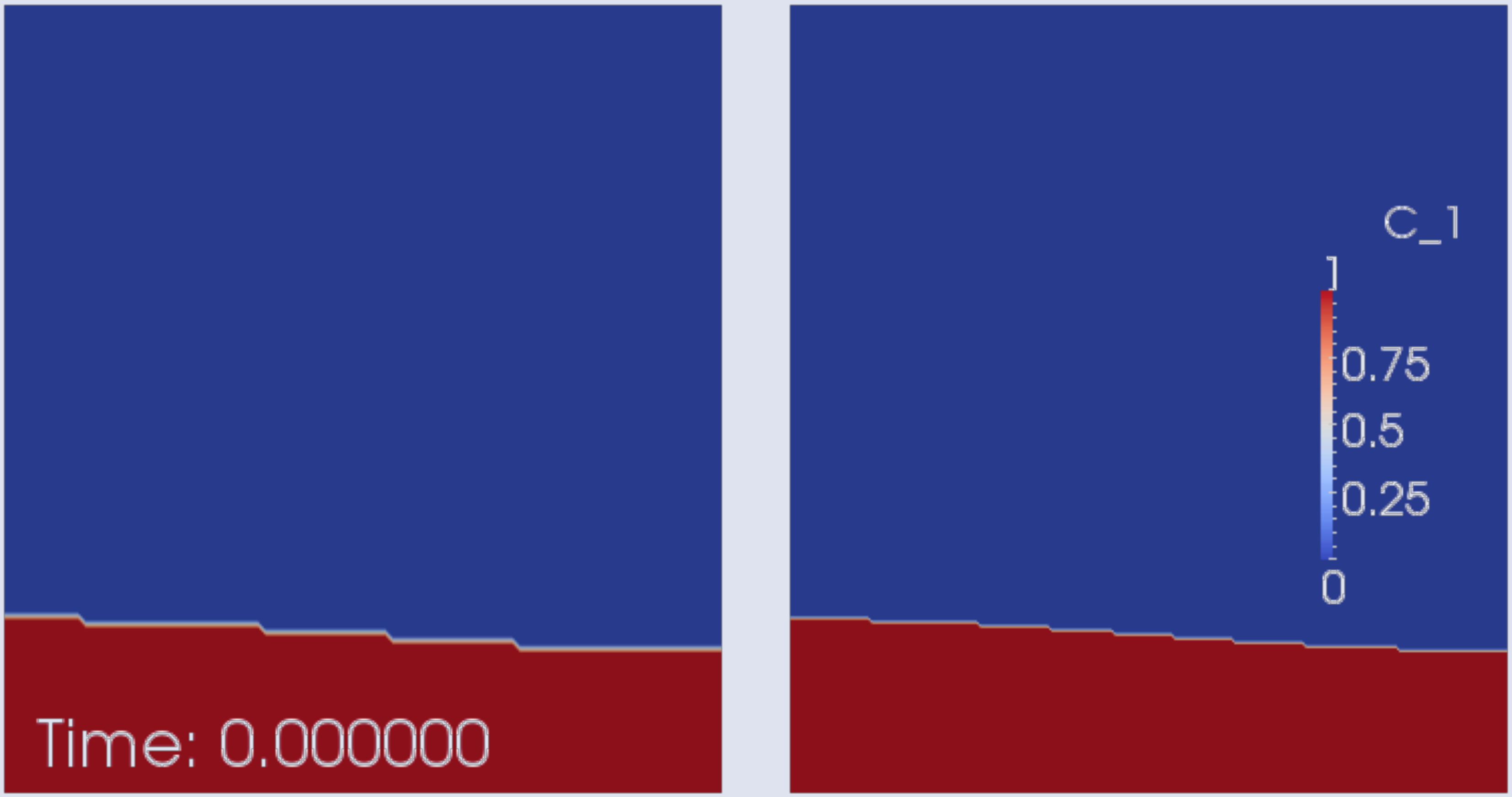
Results



Problem: No convergence!!!

Why?

Back to the initial conditions…



Change initial conditions

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
Set Output directory        = rayleigh-taylor-smooth
```

```
subsection Compositional initial conditions
  set Model name = function
  subsection Function
    set Variable names      = x,z
    set Function constants  = pi=3.14159
    set Function expression = 0.5*(1+tanh((0.2+0.02*cos(pi*x/0.9142)-z)/0.02))
  end
end
```

Running the model

aspect rayleigh_taylor.prm

Approximation by a continuous function: Interpolation over a few grid elements using a hyperbolic tangent

Visualizing results

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

1. With Paraview

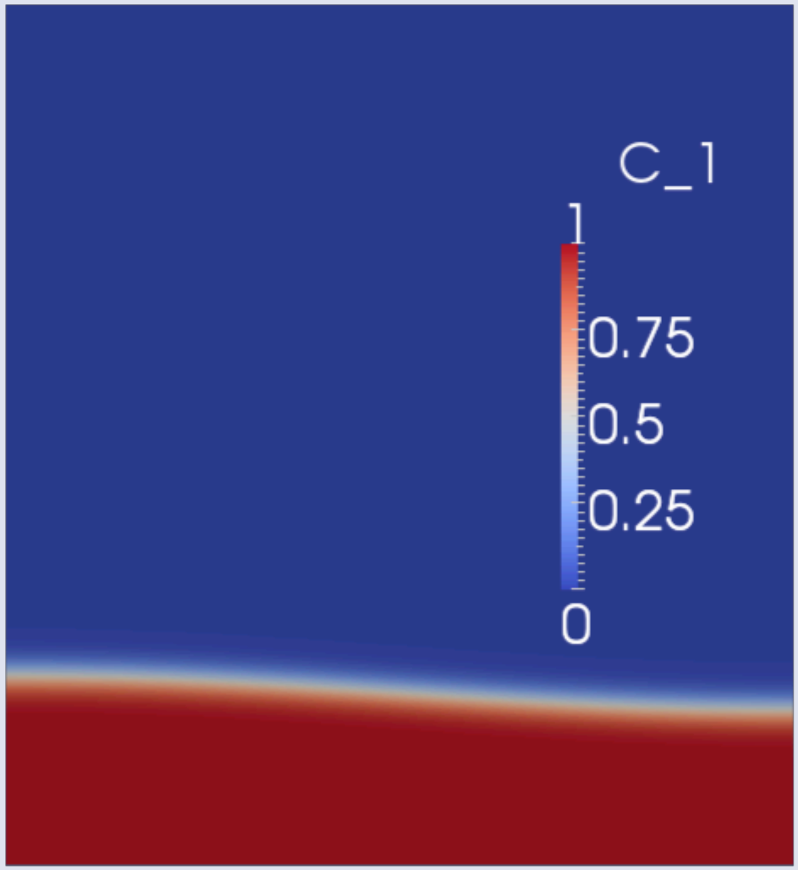
    paraview

2. With Gnuplot

    cd rayleigh-taylor-smooth
    gnuplot
    plot “statistics” using 2:14 with lines

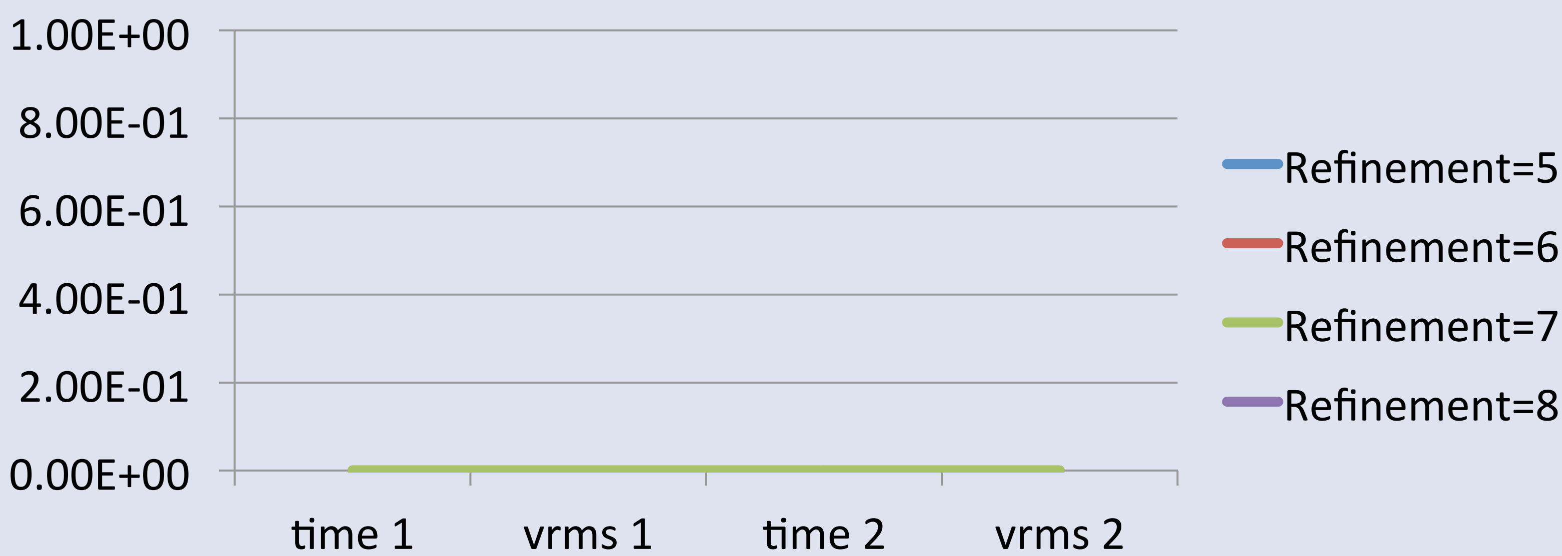
time vrms velocity

New initial conditions…



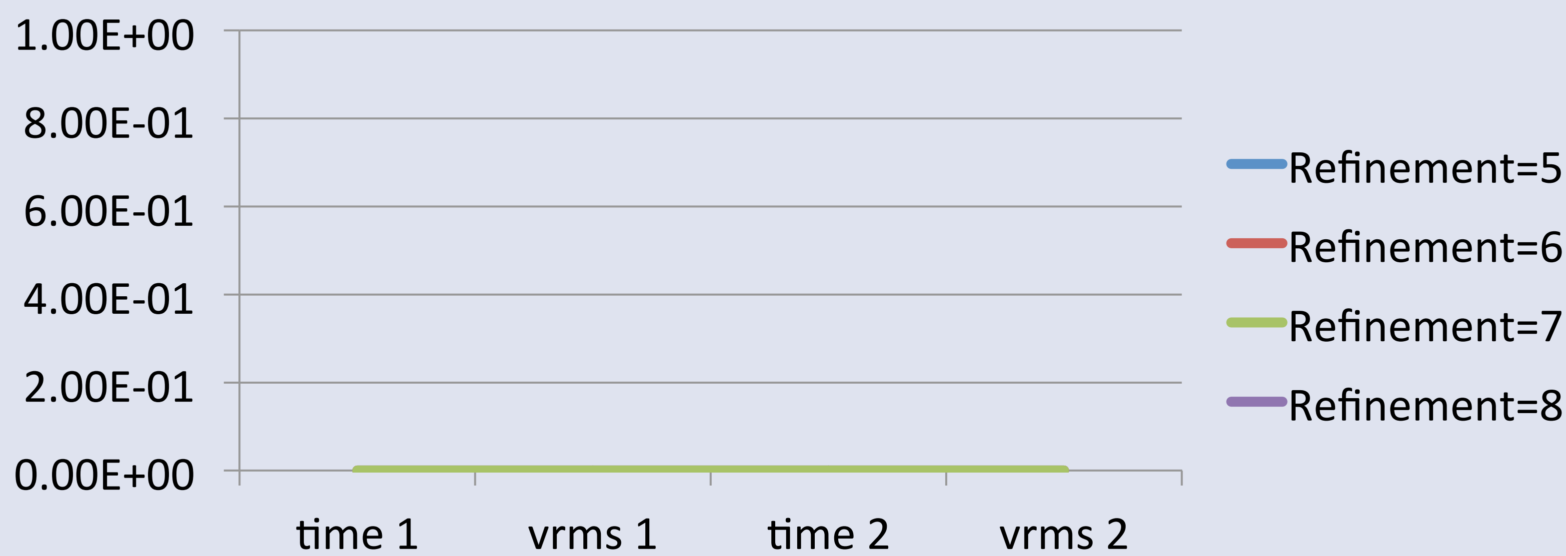
New results

	Refinement=5	Refinement=6	Refinement=7	Refinement=8
1st peak (time)	(???)	(???)	(???)	(???)
1st peak (v_{rms})	(???)	(???)	(???)	(???)
2nd peak (time)	(???)	(???)	(???)	(???)
2nd peak (v_{rms})	(???)	(???)	(???)	(???)

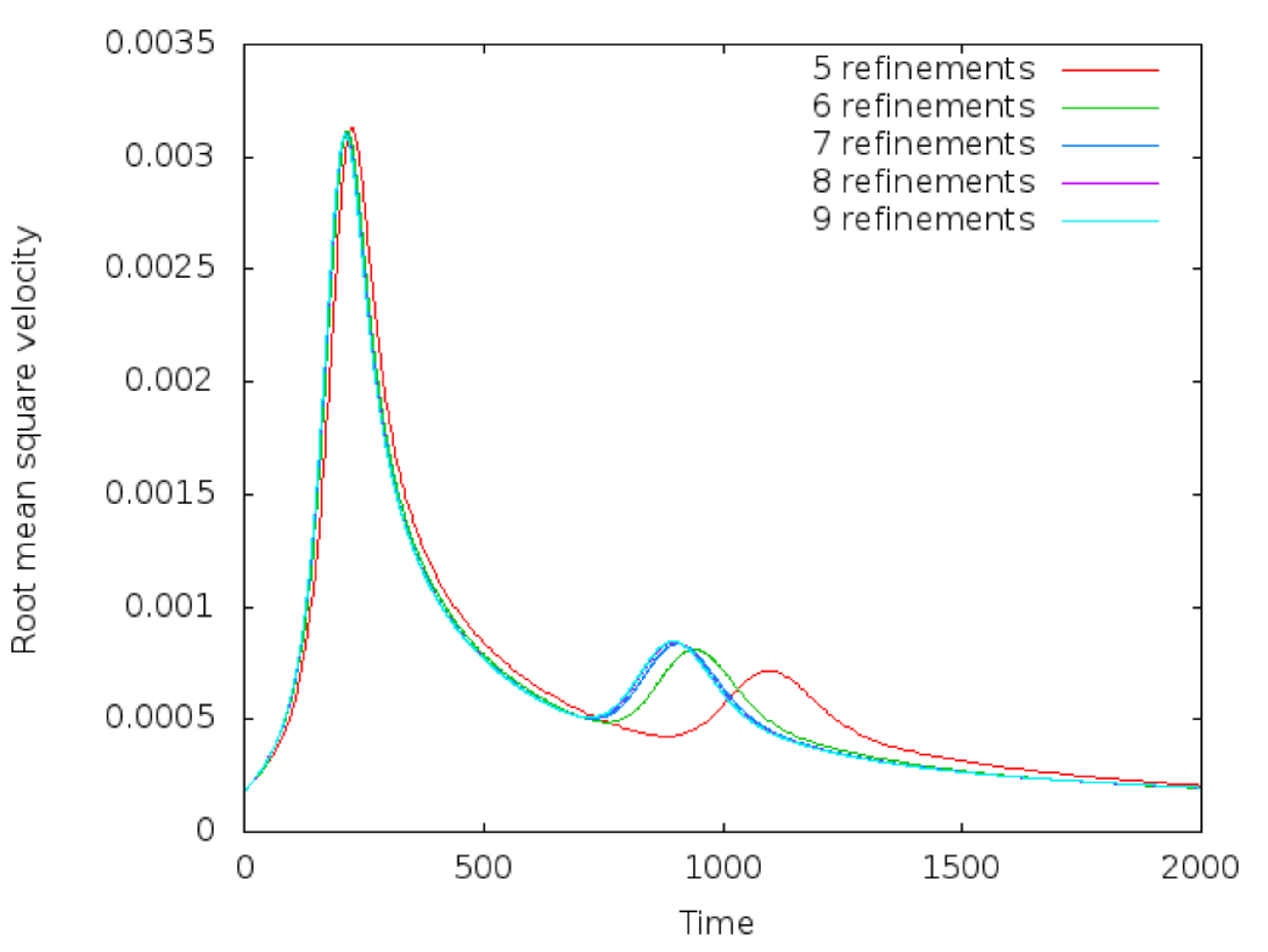


Backup slide with results

	Refinement=5	Refinement=6	Refinement=7	Refinement=8
1st peak (time)	(???)	(???)	(???)	(???)
1st peak (v_{rms})	(???)	(???)	(???)	(???)
2nd peak (time)	(???)	(???)	(???)	(???)
2nd peak (v_{rms})	(???)	(???)	(???)	(???)



Convergence

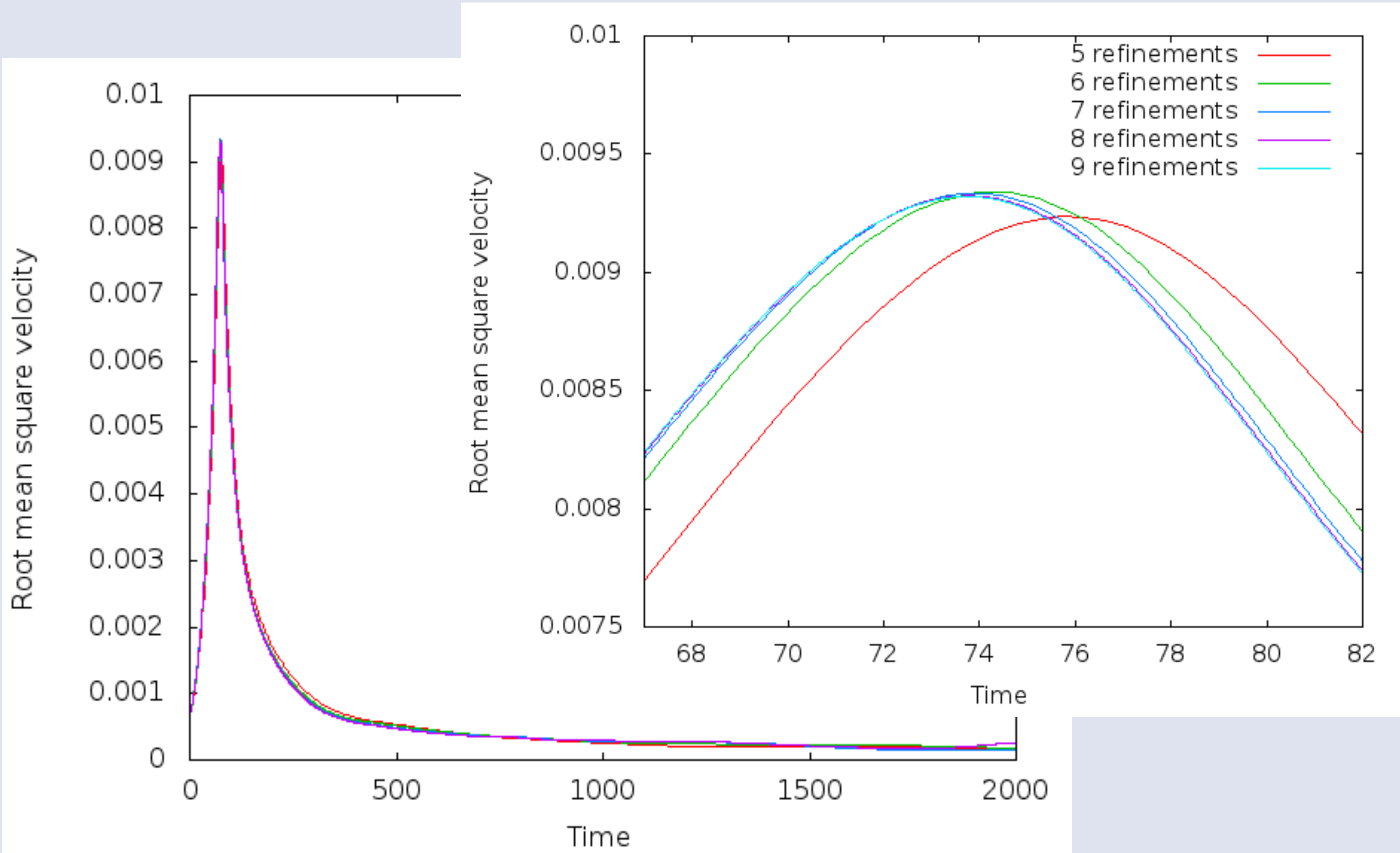


Variable viscosity

```
subsection Material model
  set Model name = simple
  subsection Simple model
    set Viscosity                                          = 1e2
    set Thermal expansion coefficient                      = 0
    set Density differential for compositional field 1 = -10
    set Composition viscosity prefactor                    = 0.1
  end
end
```

10x reduced viscosity in the lower layer

Results


0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
Root mean square velocity
0
500
1000
1500
2000
Time
0.01
0.0095
0.009
0.0085
0.008
0.0075
Root mean square velocity
68
70
72
74
76
78
80
82
Time
5 refinements
6 refinements
7 refinements
8 refinements
9 refinements