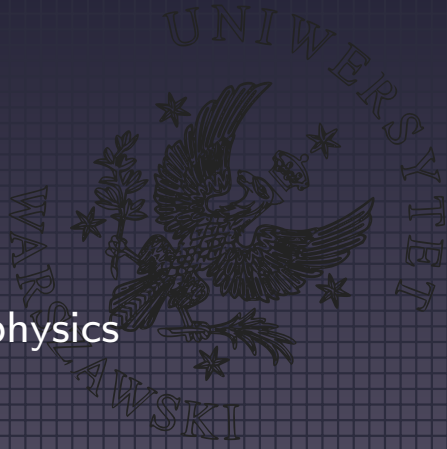
icicle

http://icicle.igf.fuw.edu.pl/

a new MPDATA-based solver for systems of transport equations with emphasis on cloud modelling

Sylwester Arabas
Anna Jaruga
Hanna Pawłowska

University of Warsaw / Faculty of Physics / Institute of Geophysics



8th International Cloud Modelling Workshop, Warsaw, 26th July 2012

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Why develop

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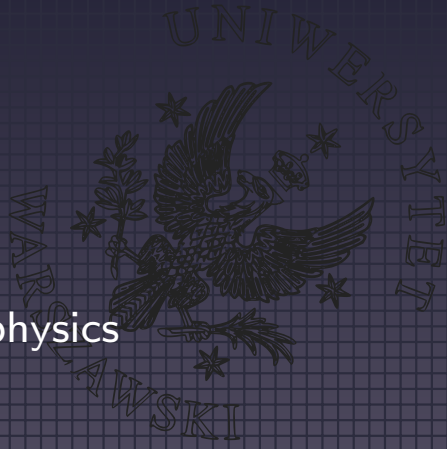

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rationale behind icicle

$$\partial_t \psi_i + \nabla \cdot (\vec{v} \psi_i) = R_i$$

- systems of advective transport (continuity) equations pop up frequently in geosciences ⇝ need for accurate & efficient solvers
- MPDATA (Smolarkiewicz 1983, ...) is:
  - second-order accurate in space and time
  - multidimensional and sign-preserving by design
  - optionally non-oscillatory (flux-corrected transport)
  - iterative ⇝ readily parallelisable
  - traditionally the solver-of-choice at the University of Warsaw :)
- there's no implementation of an MPDATA-based solver that:
  - is free (as in free speech) and open-source
  - has technical documentation (re-usability)
  - uses object-oriented programming (OOP)

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OOP vs. MPDATA

$$\psi_{i,j}^{[n+1]} = \psi_{i,j}^{[n]} - \sum_{d=0}^{N-1} \left(F\left[\psi^{[n]}_{\pi^d_{i,j}}, \psi^{[n]}_{\pi^d_{i+1,j}}, C^{[d]}_{\pi^d_{i+1/2,j}} \right] - F\left[\psi^{[n]}_{\pi^d_{i-1,j}}, \psi^{[n]}_{\pi^d_{i,j}}, C^{[d]}_{\pi^d_{i-1/2,j}} \right] \right)$$

1D donor-cell in C++/Blitz++

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template <class pi>
inline auto donorcell_1D(
  const arr_t &psi,
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) return_macro(
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2D donor-cell in C++/Blitz++

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inline void donorcell_2D(
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) {
  psi[n+1](i,j) = psi[n](i,j)
    - donorcell_1D<pi_ij>(psi[n], C[0], i, j)
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Arakawa-C grid with operator overloading

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struct hlf_t {} h;

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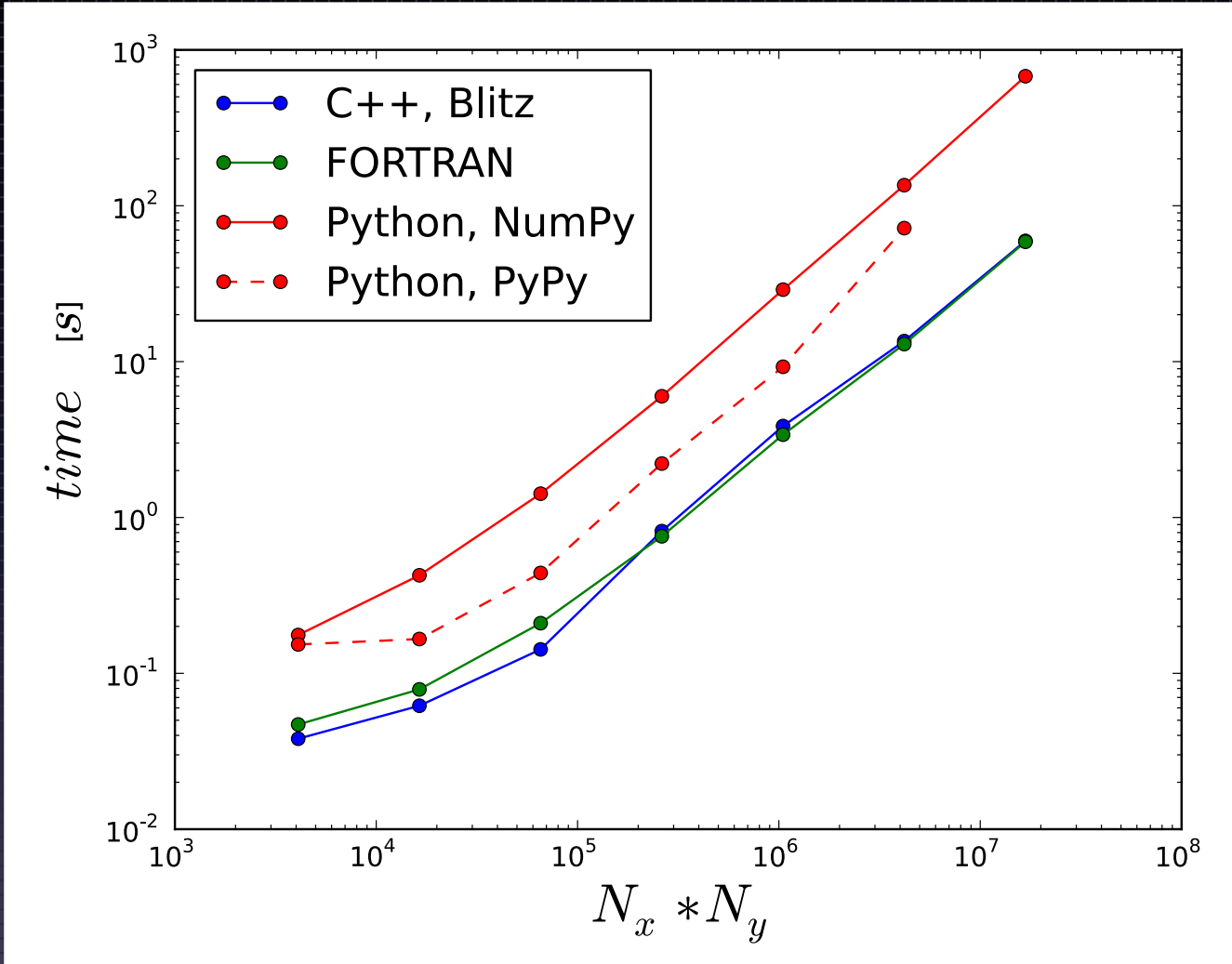
C++ vs. FORTRAN vs. Python: performance



donor-cell times from Jarecka et al. 2012 EGU poster
MPDATA paper in preparation

C++ can check units for you (at no runtime cost!)

κ-Köhler parameterisation

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  /// @brief activity of water in solution
  /// (eqs. 1,6) in @copydetails Petters_and_Kreidenweis_2007
  template <typename real_t>
  quantity<si::dimensionless, real_t> a_w(
    quantity<si::volume, real_t> rw3,
    quantity<si::volume, real_t> rd3,
    quantity<si::dimensionless, real_t> kappa
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  {
    return (rw3 - rd3) / (rw3 - rd3 * (real_t(1) - kappa));
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$\rightsquigarrow$ Boost.units

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- human-readable + open-source $\rightsquigarrow$ auditable (code review!)
- shorter $\rightsquigarrow$ less bug-prone, easier to debug
- reusable $\rightsquigarrow$ coding time savings in the long run
- shareable $\rightsquigarrow$ common libraries instead of copy-paste!
- maintainable $\rightsquigarrow$ less bug-prone, easier to co-operate on
- modular $\rightsquigarrow$ full separation of numerics/physics/concurrency/io
- optimisable (by the compiler/library author) $\rightsquigarrow$ potentially faster

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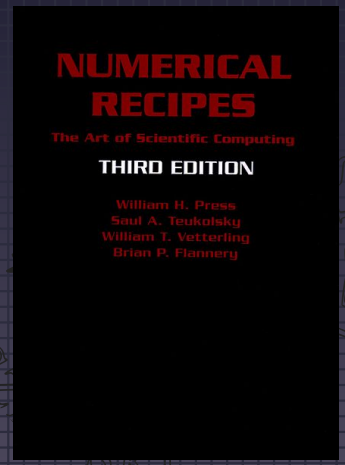
- maintainable $\rightsquigarrow$ less bug-prone, easier to co-operate on
- modular $\rightsquigarrow$ full separation of numerics/physics/concurrency/io
- optimisable (by the compiler/library author) $\rightsquigarrow$ potentially faster

the aims of icicle

"[Object oriented programming] has become recognised as the almost unique successful paradigm for creating complex software"

NR: The Art of Scientific Computing (3rd ed., Press et al. 2007)



icicle

http://icicle.igf.fuw.edu.pl/

Why develop

a new MPDATA-based solver for systems of transport equations with emphasis on cloud modelling

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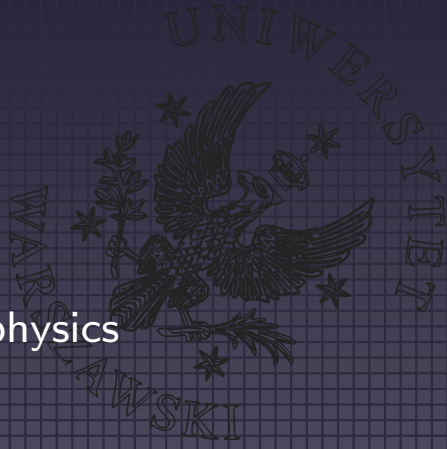
Sylwester Arabas
Anna Jaruga
Hanna Pawłowska

University of Warsaw / Faculty of Physics / Institute of Geophysics



8th International Cloud Modelling Workshop, Warsaw, 26th July 2012

icicle

http://icicle.igf.fuw.edu.pl/

Why develop
a new MPDATA-based solver for systems of transport equations with emphasis on cloud modelling
and what one may already do with it?

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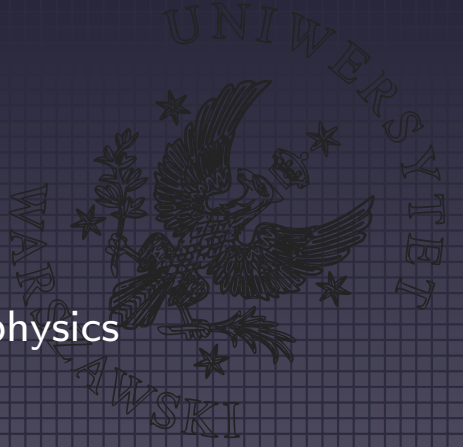

8th International Cloud Modelling Workshop, Warsaw, 26th July 2012

icicle: currently available components

- advection scheme:
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    - any number of iterations
    - 3^{rd} order accuracy option
    - FCT (aka non-oscillatory) option
    - variable-sign field option
  - donor-cell, leapfrog, ...
- equation sets:
  - 2D, 3D isentropic
  - 2D moist kinematic (this workshop's "case 1")
    - bulk (Kessler) μ-physics
    - particle-based (super-droplet) μ-physics
- input/output: ASCII, netCDF-4

all selectable at runtime via command-line options

$\rightsquigarrow$ command-line string unambiguously defines simulation (in output file)

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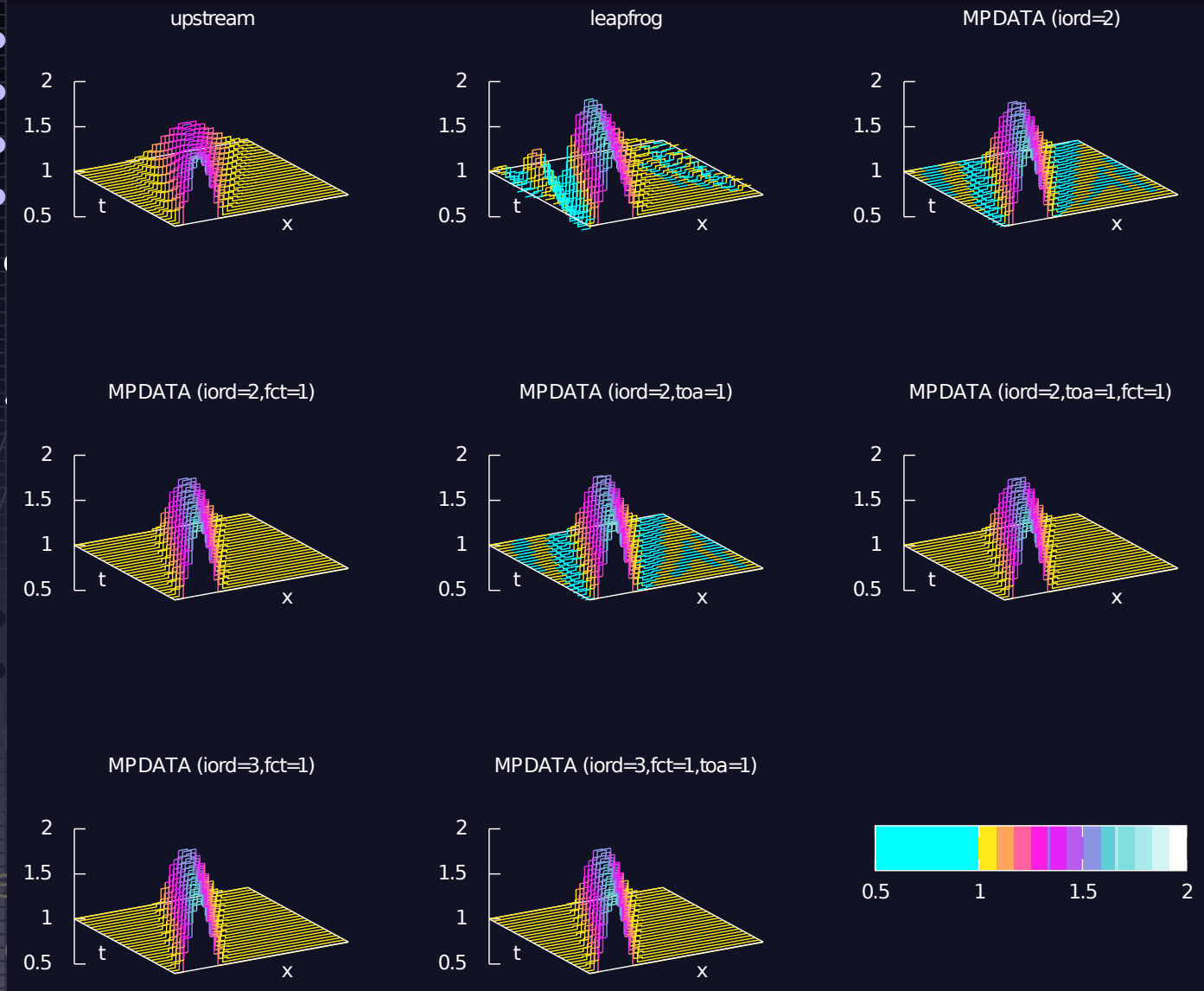
1D scalar advection examples



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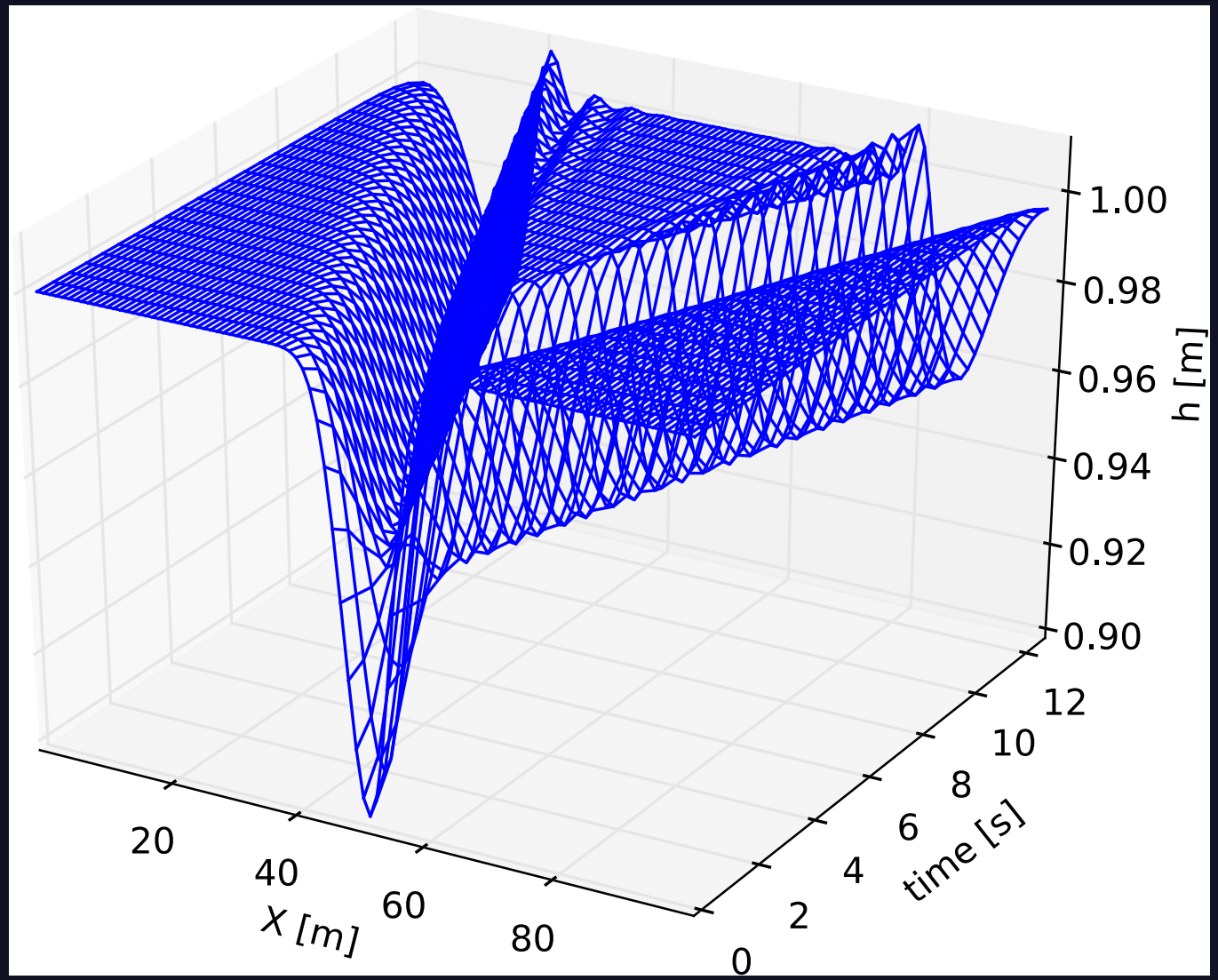
1D shallow water example



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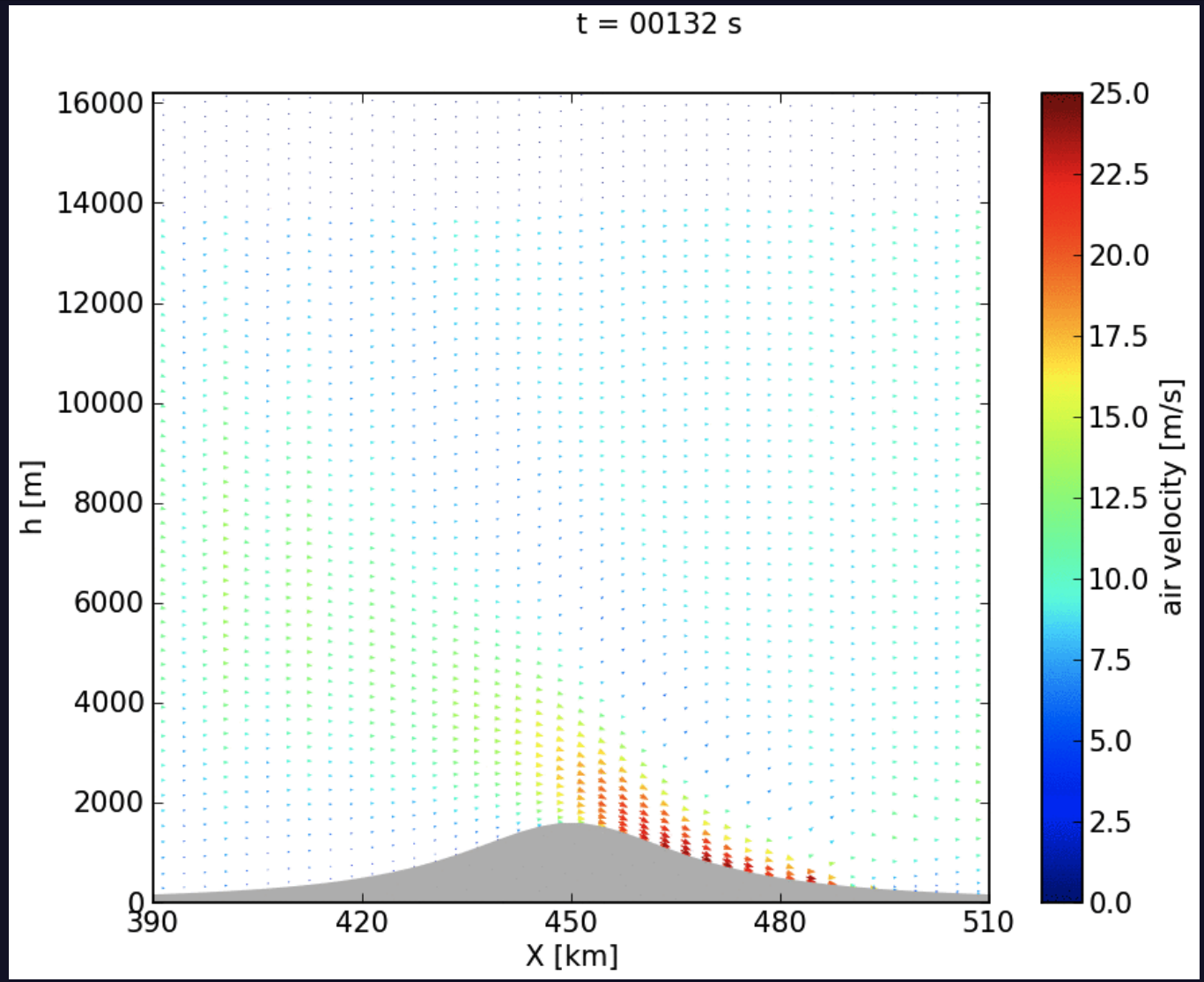
2D isentropic example



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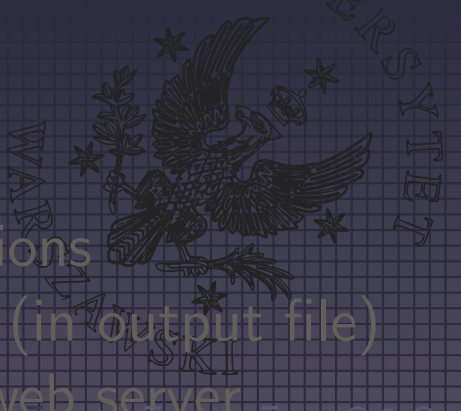

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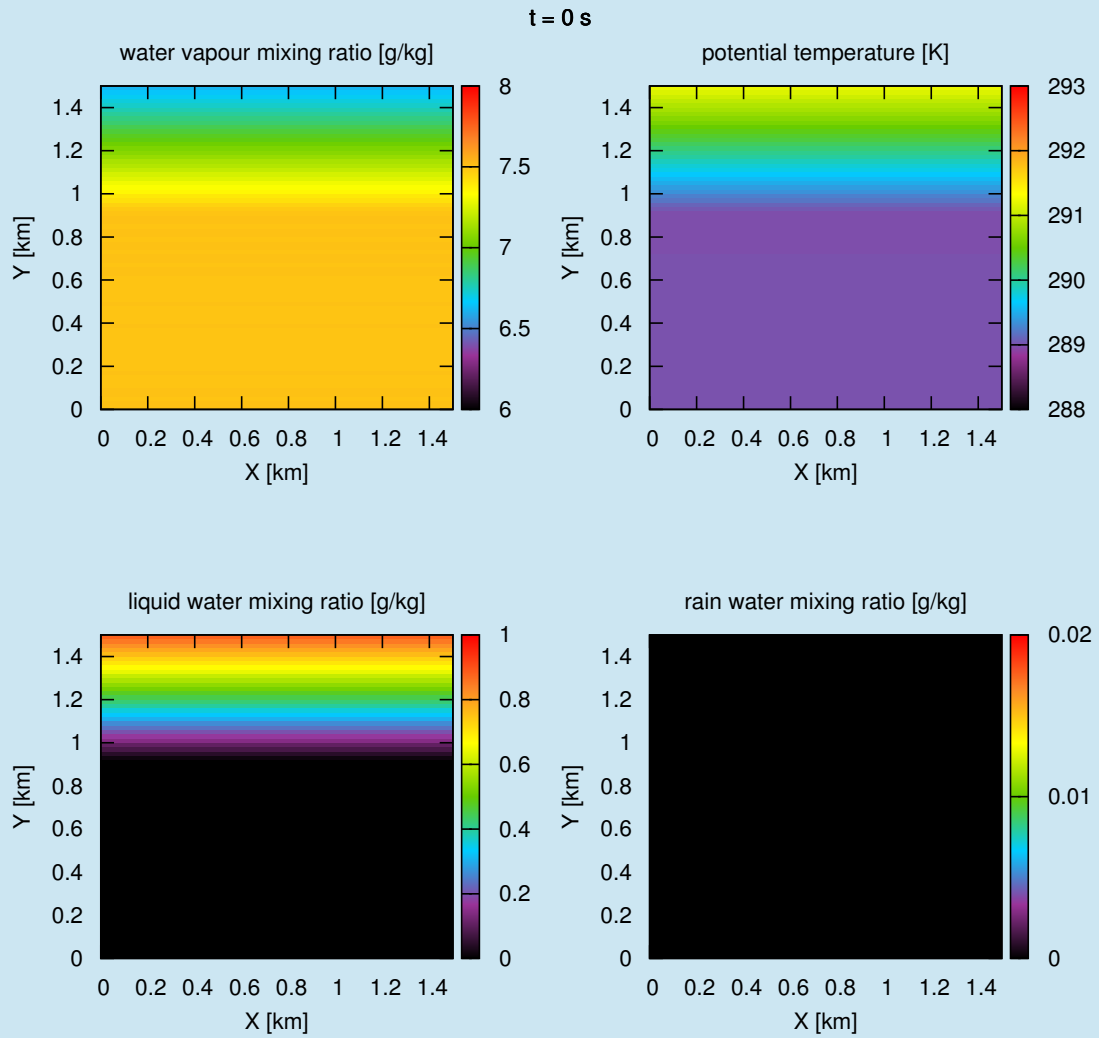
2D moist kinematic example (bulk)



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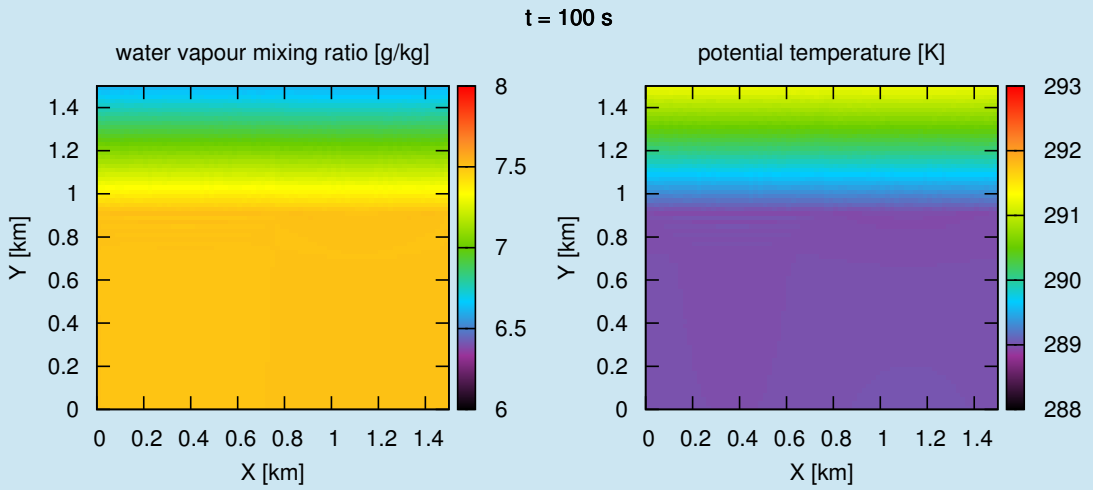

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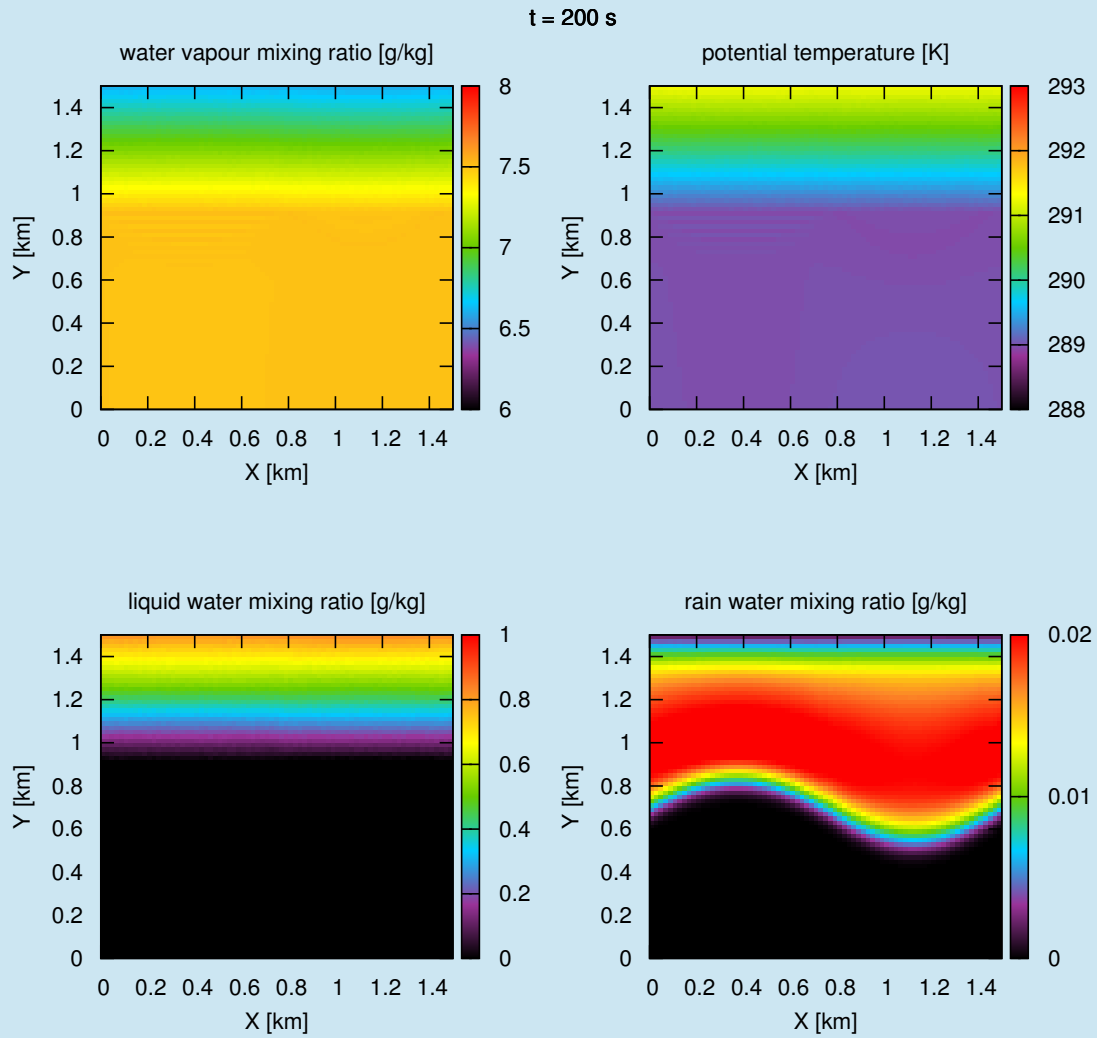

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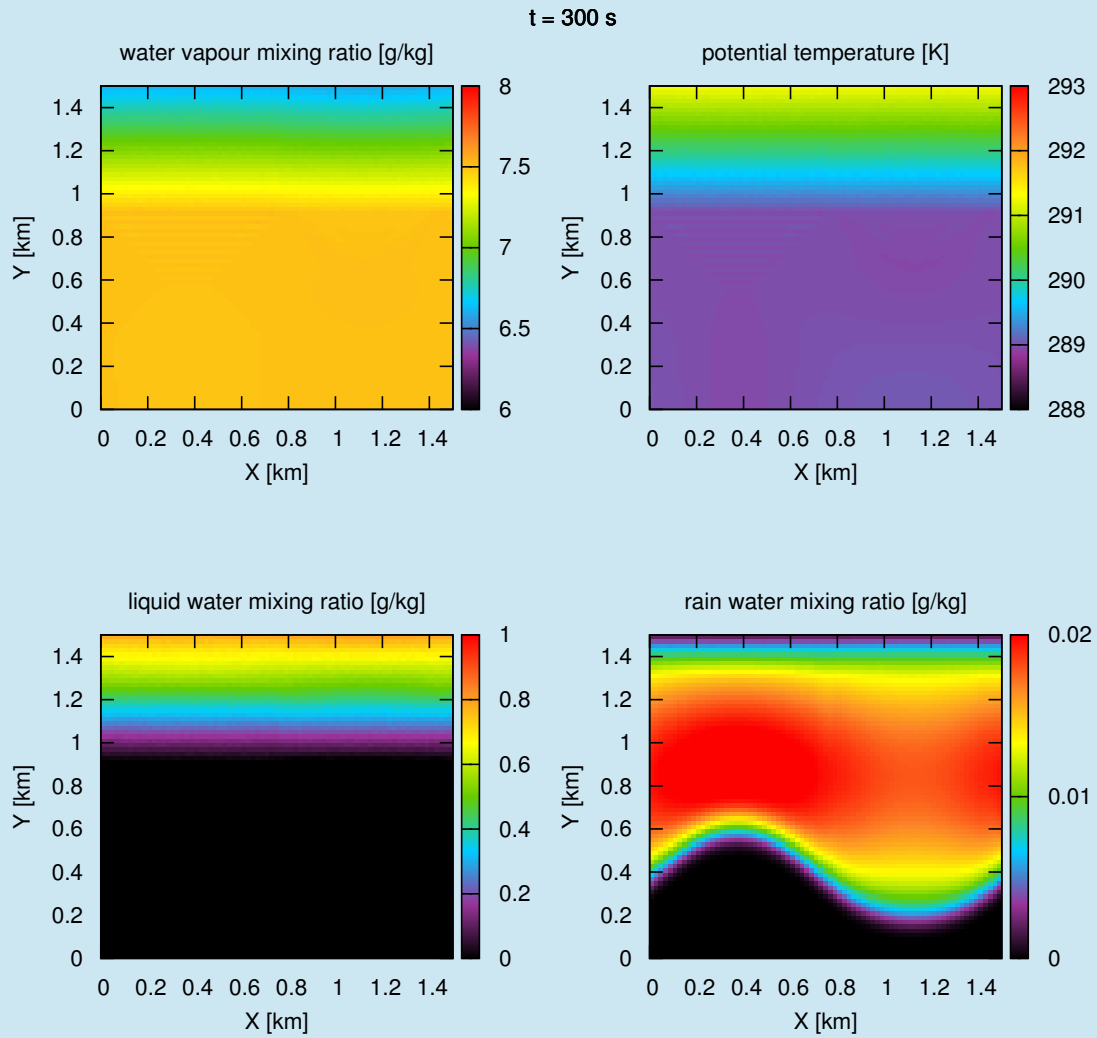

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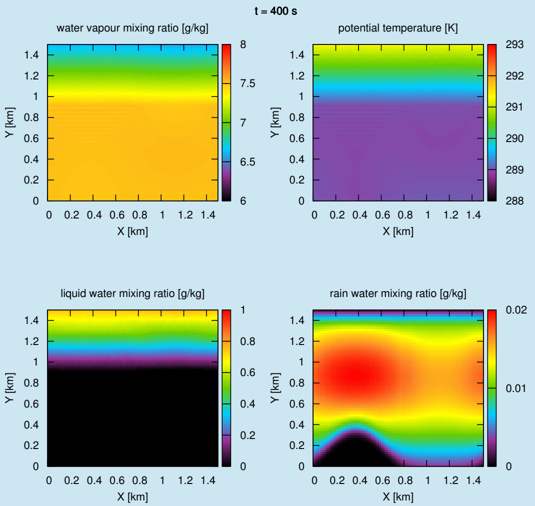

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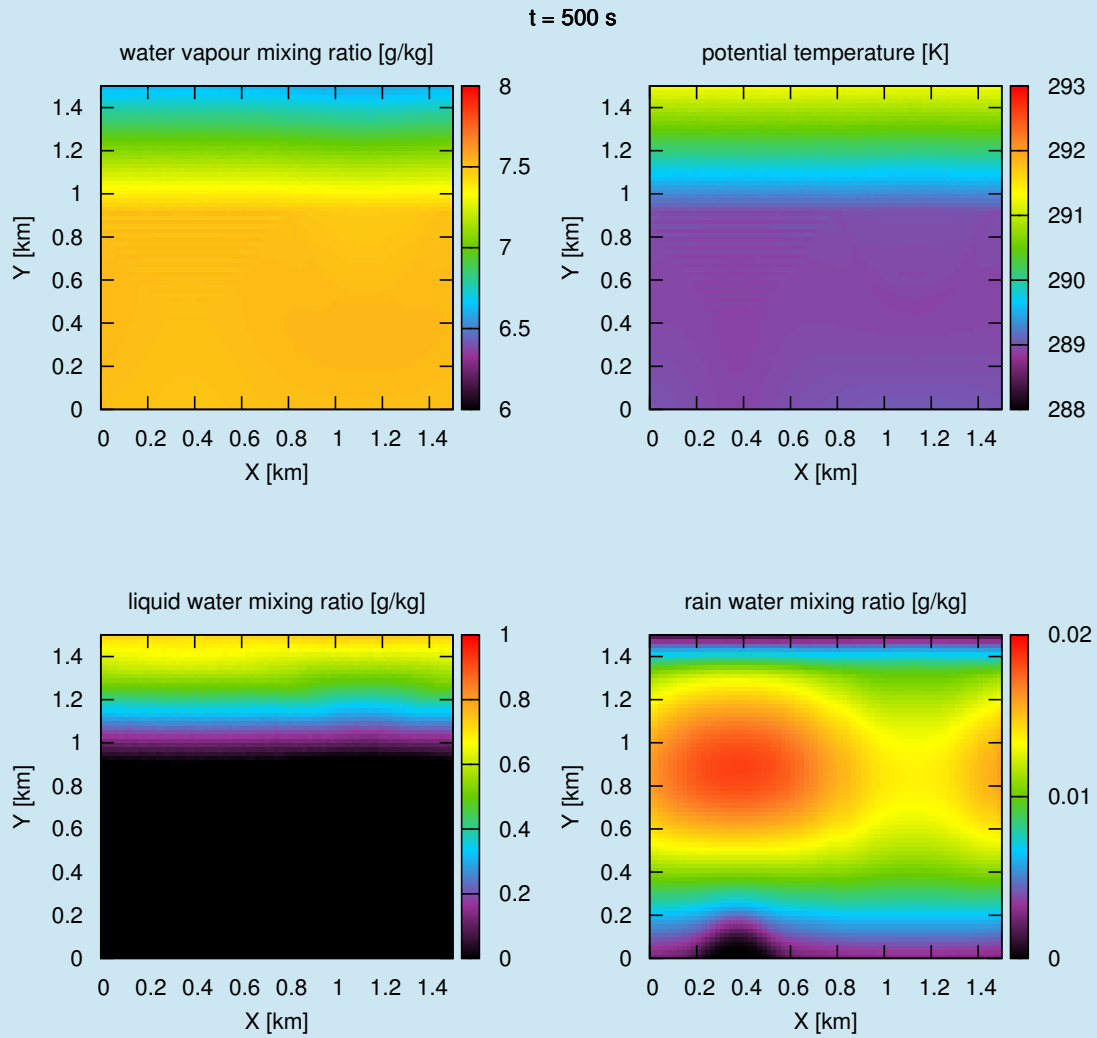

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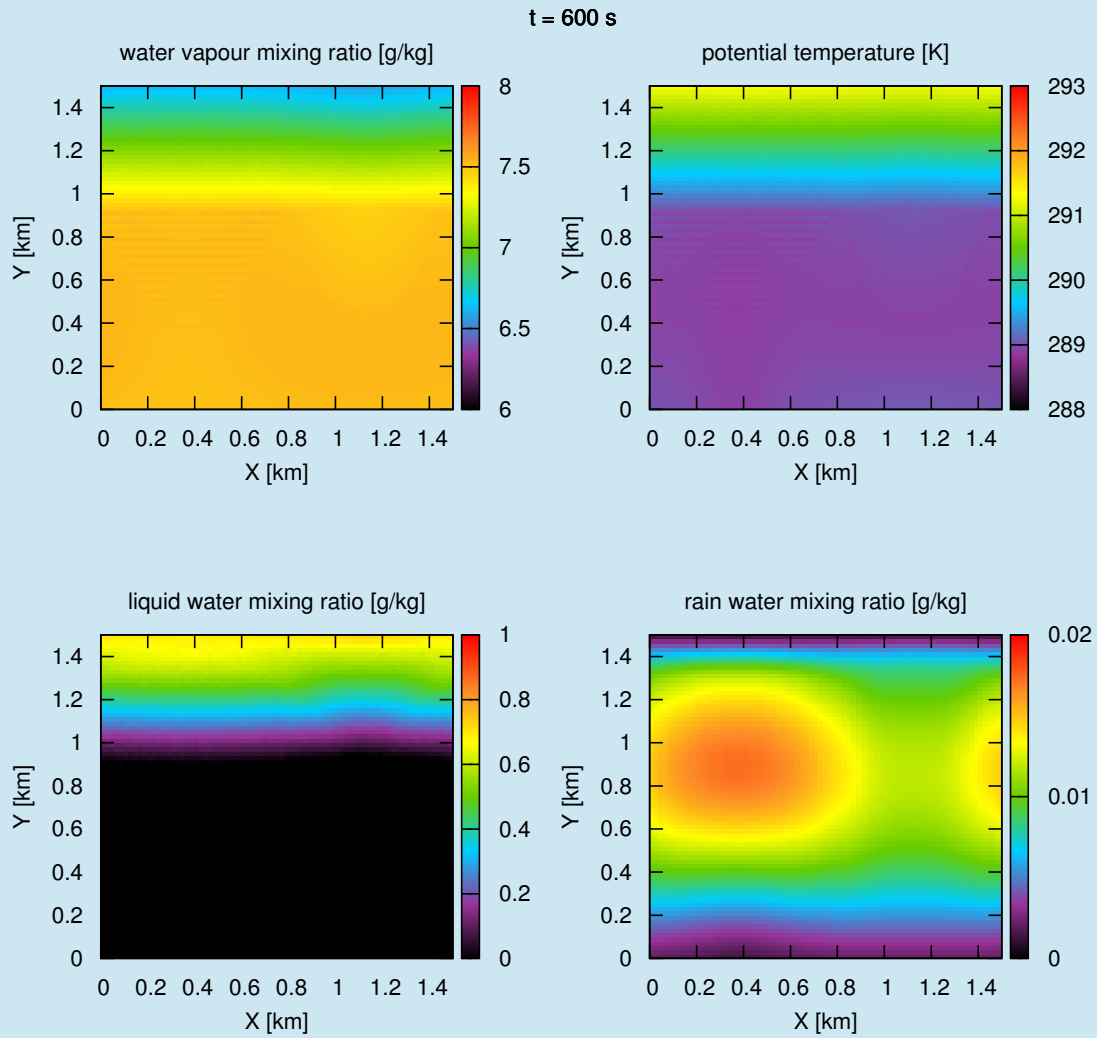

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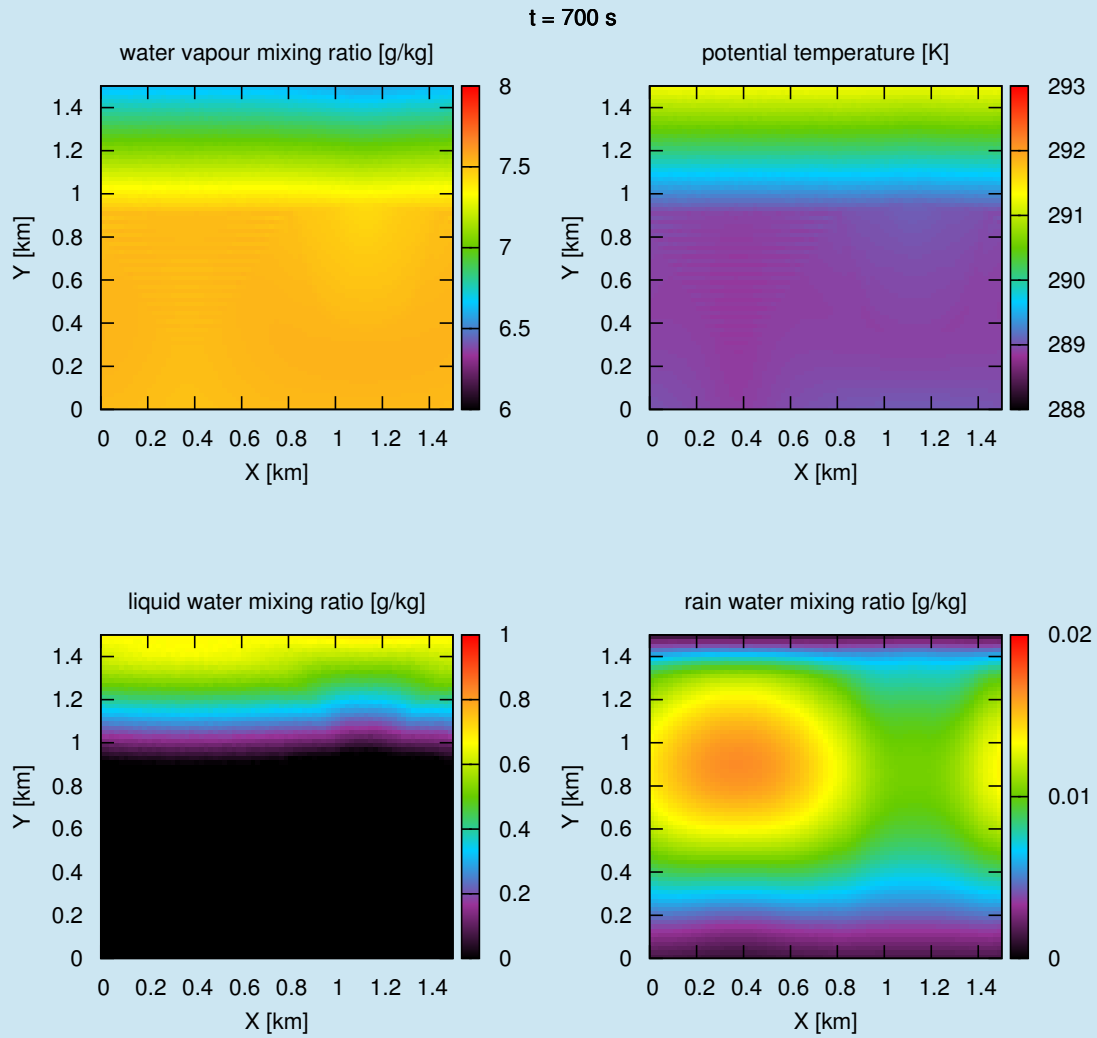

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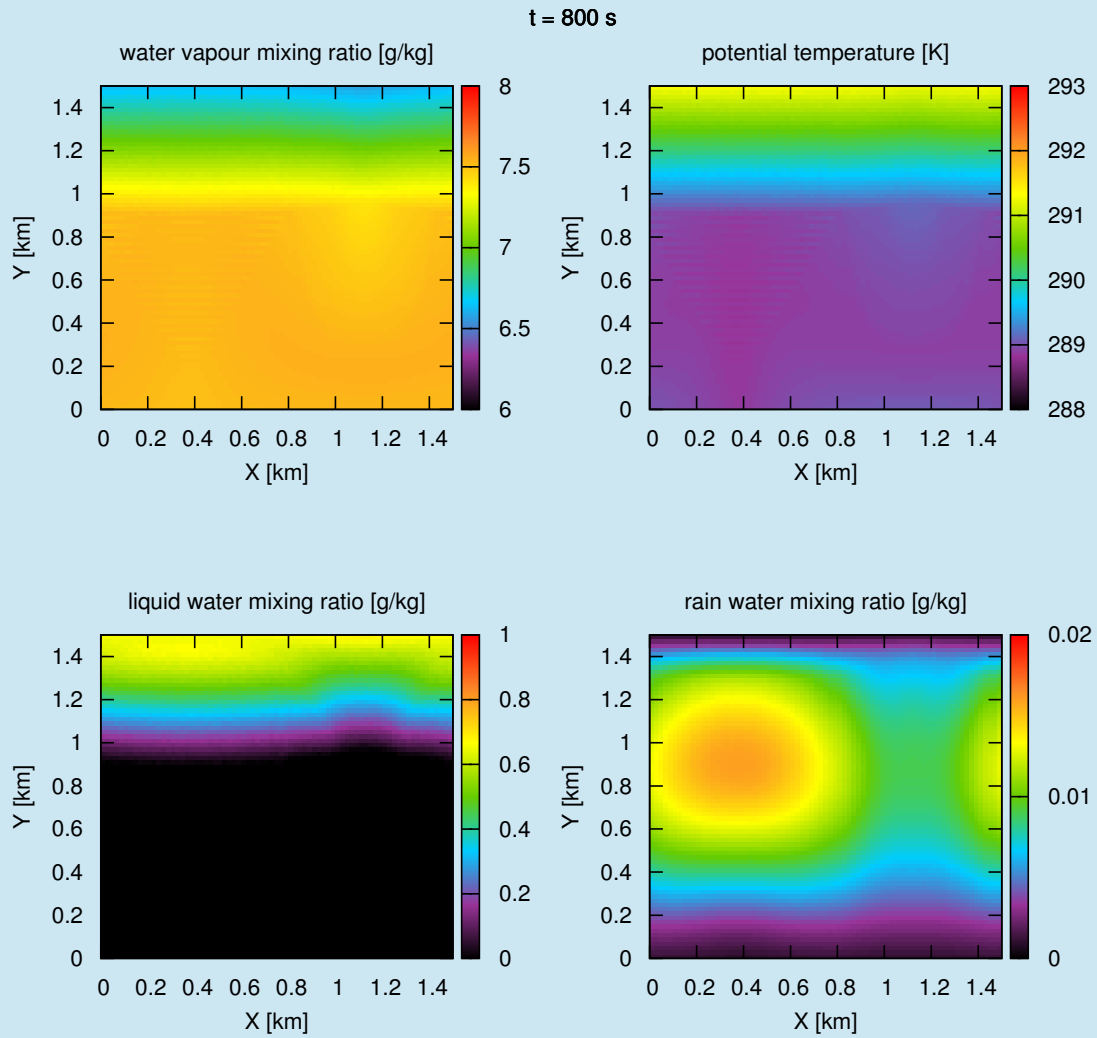

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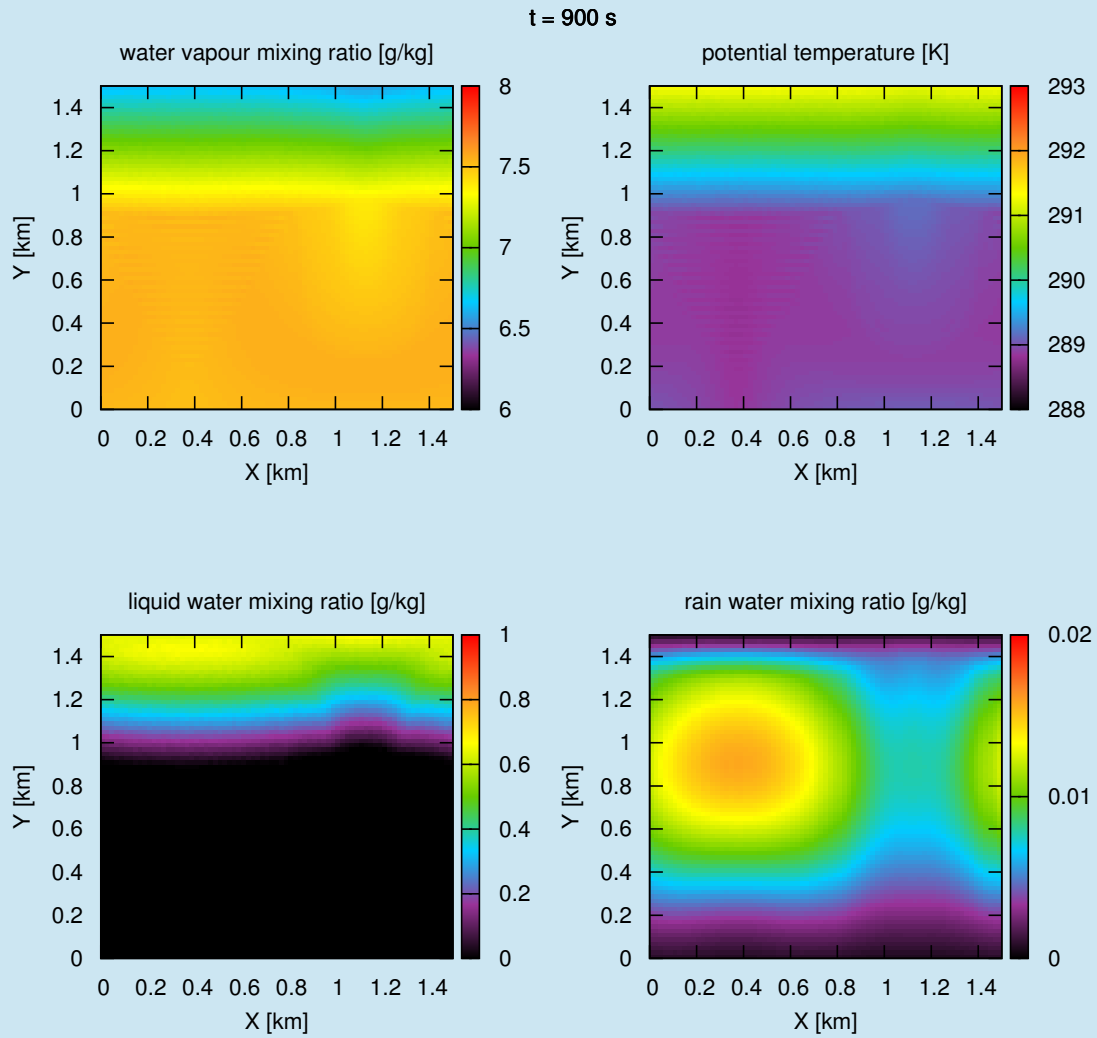

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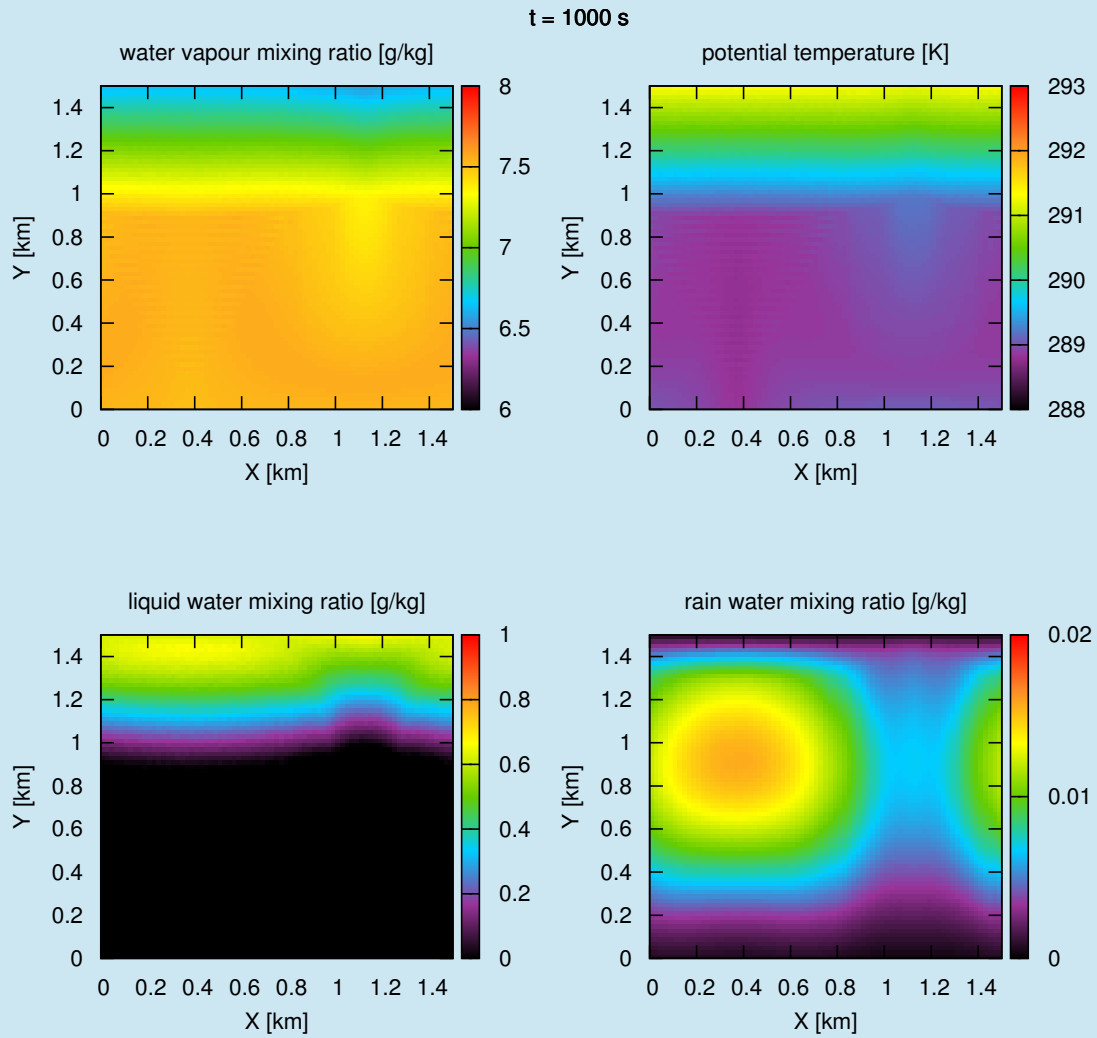

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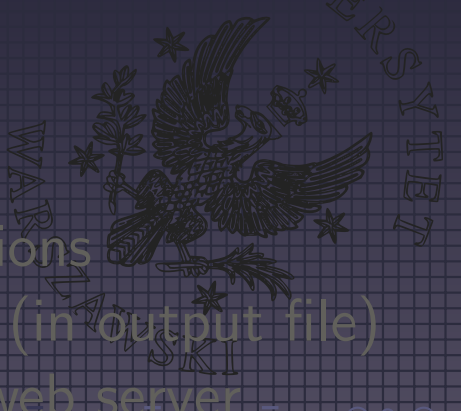

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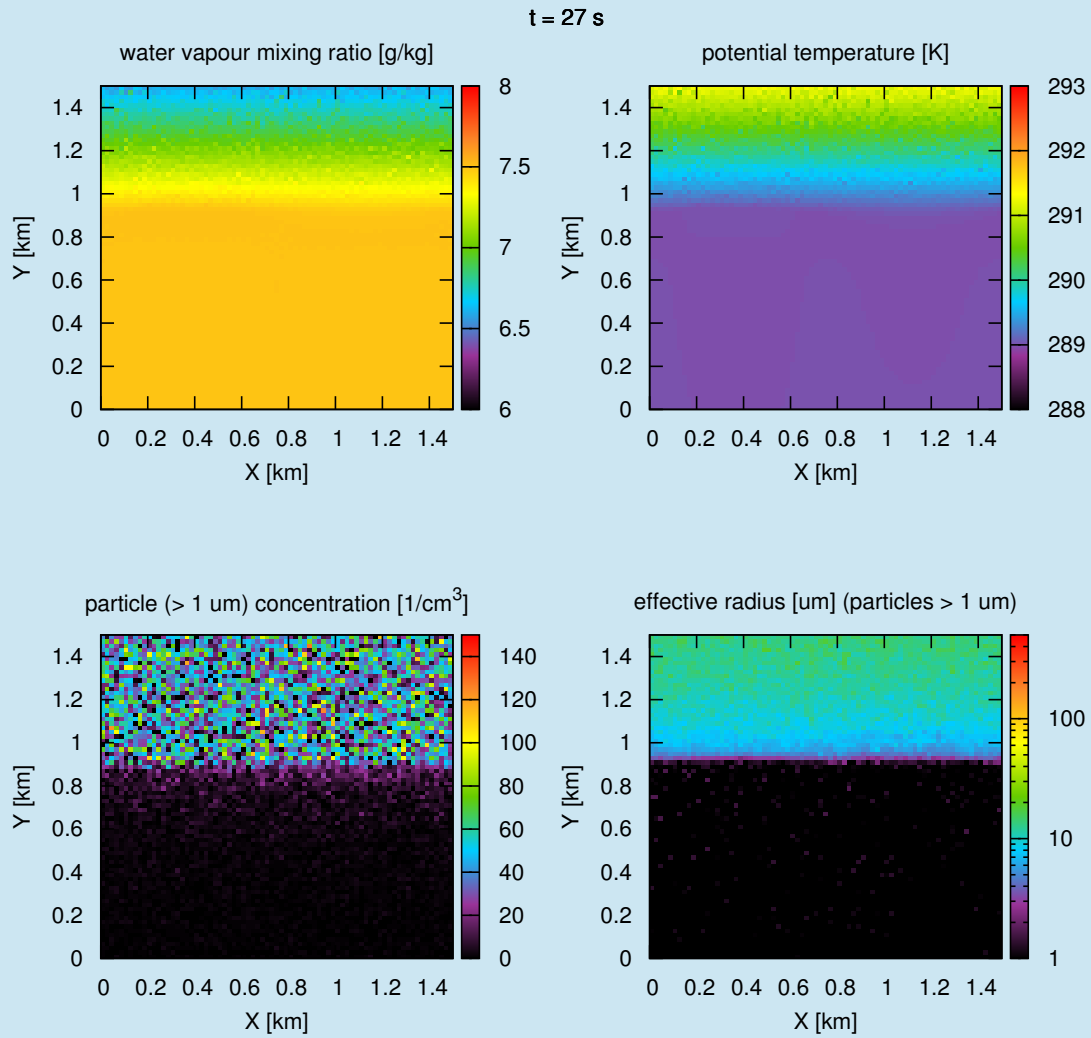

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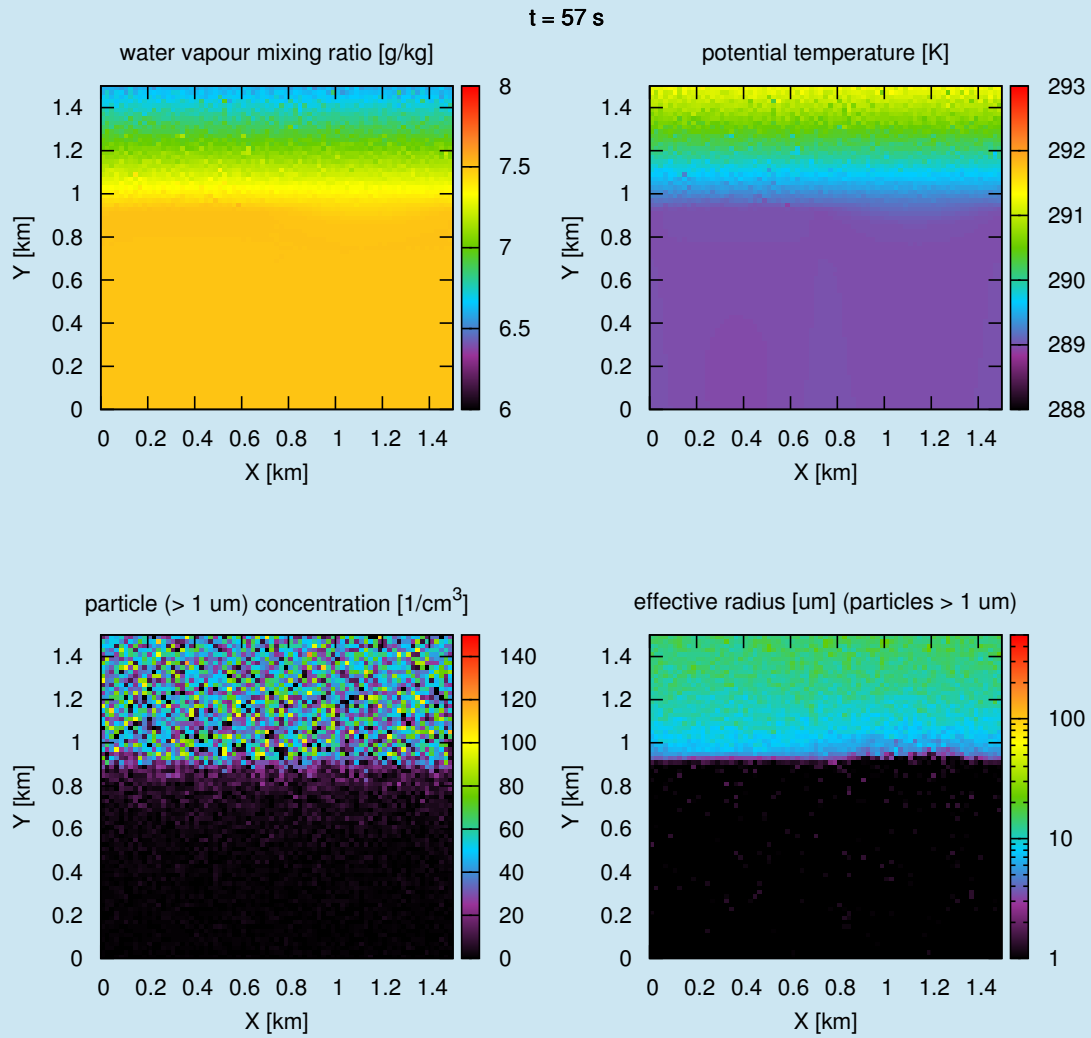

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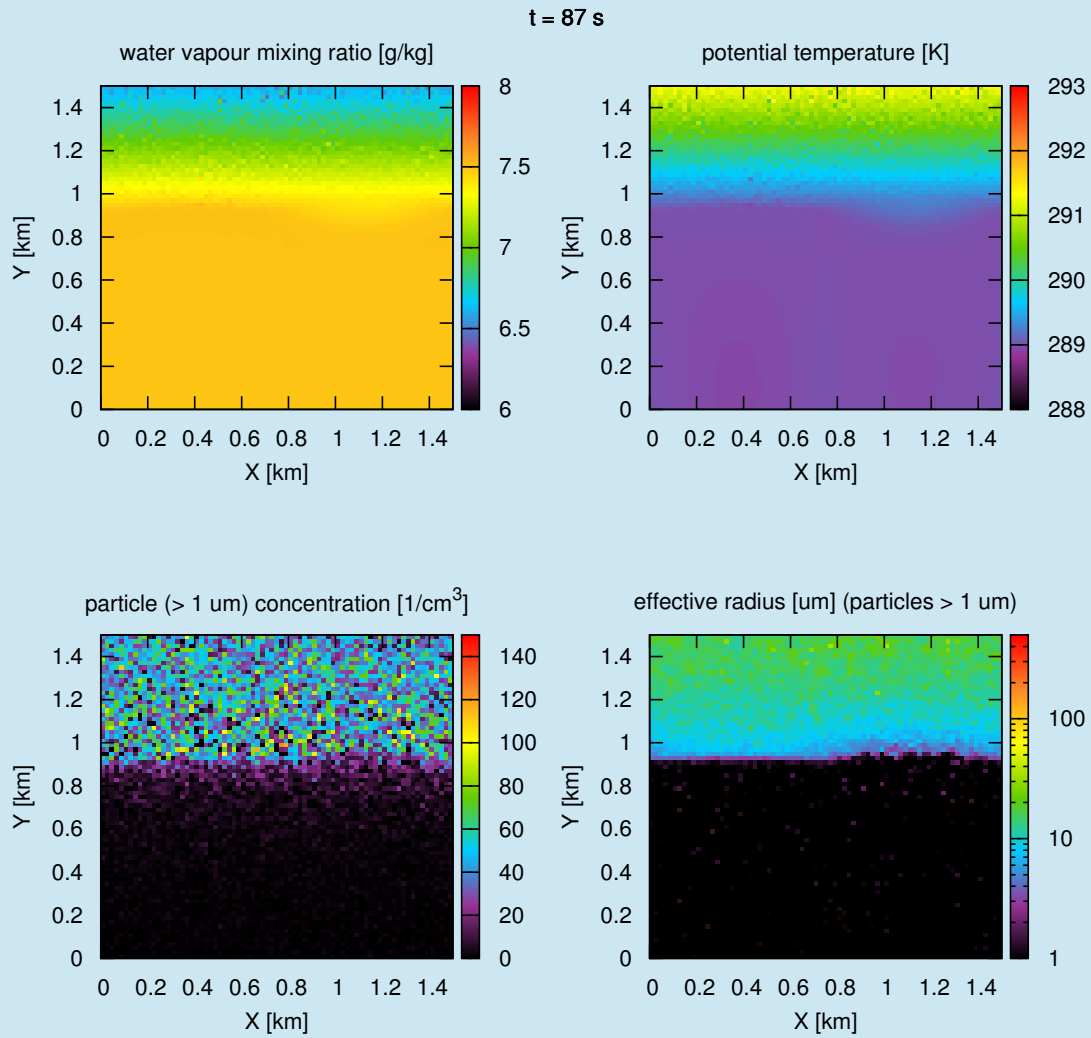

icicle: currently available components

- advection scheme:
  - MP
    - don
- equation
  - scal
  - 1D/
  - 2D/
  - 2D
- input/ou

all se

⇝ command-lin (output file)

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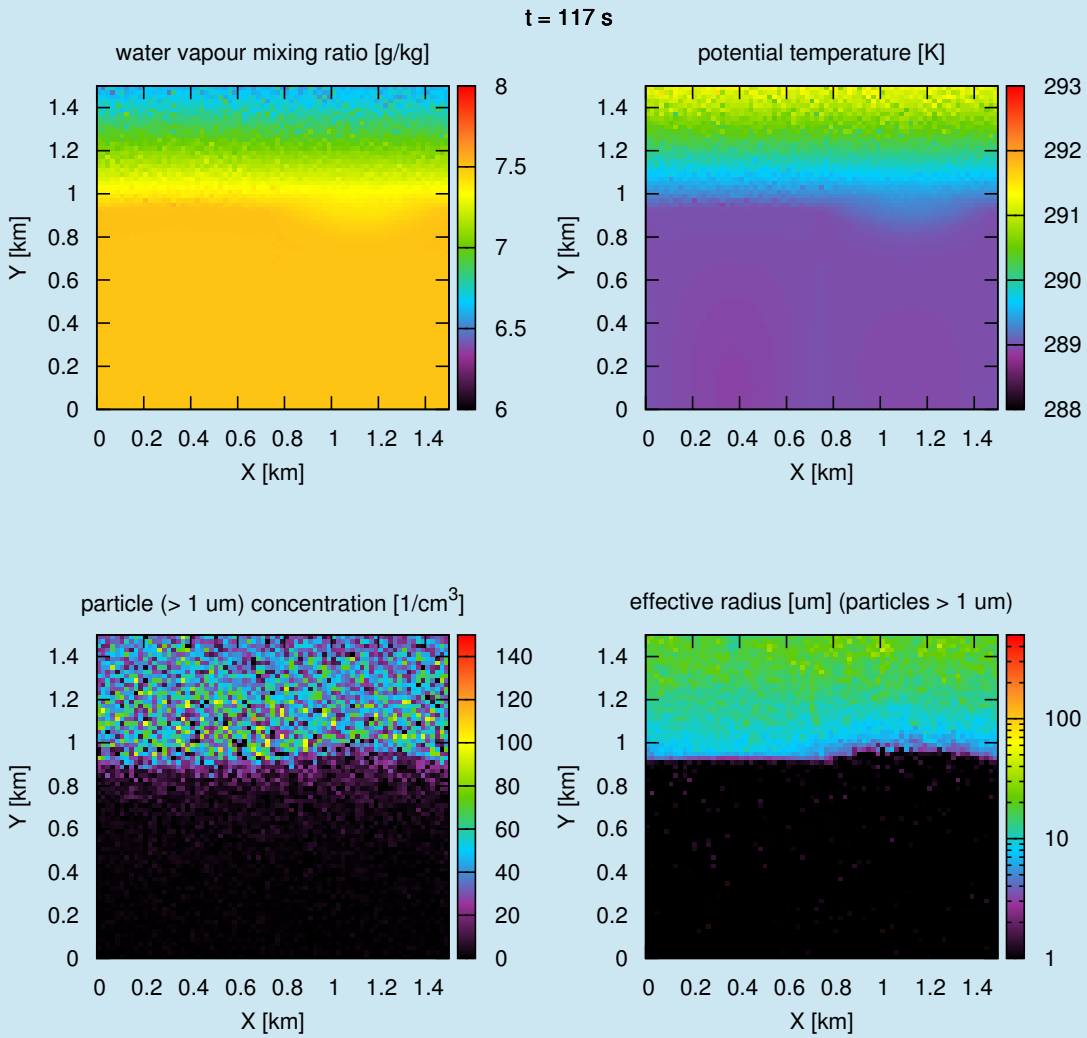

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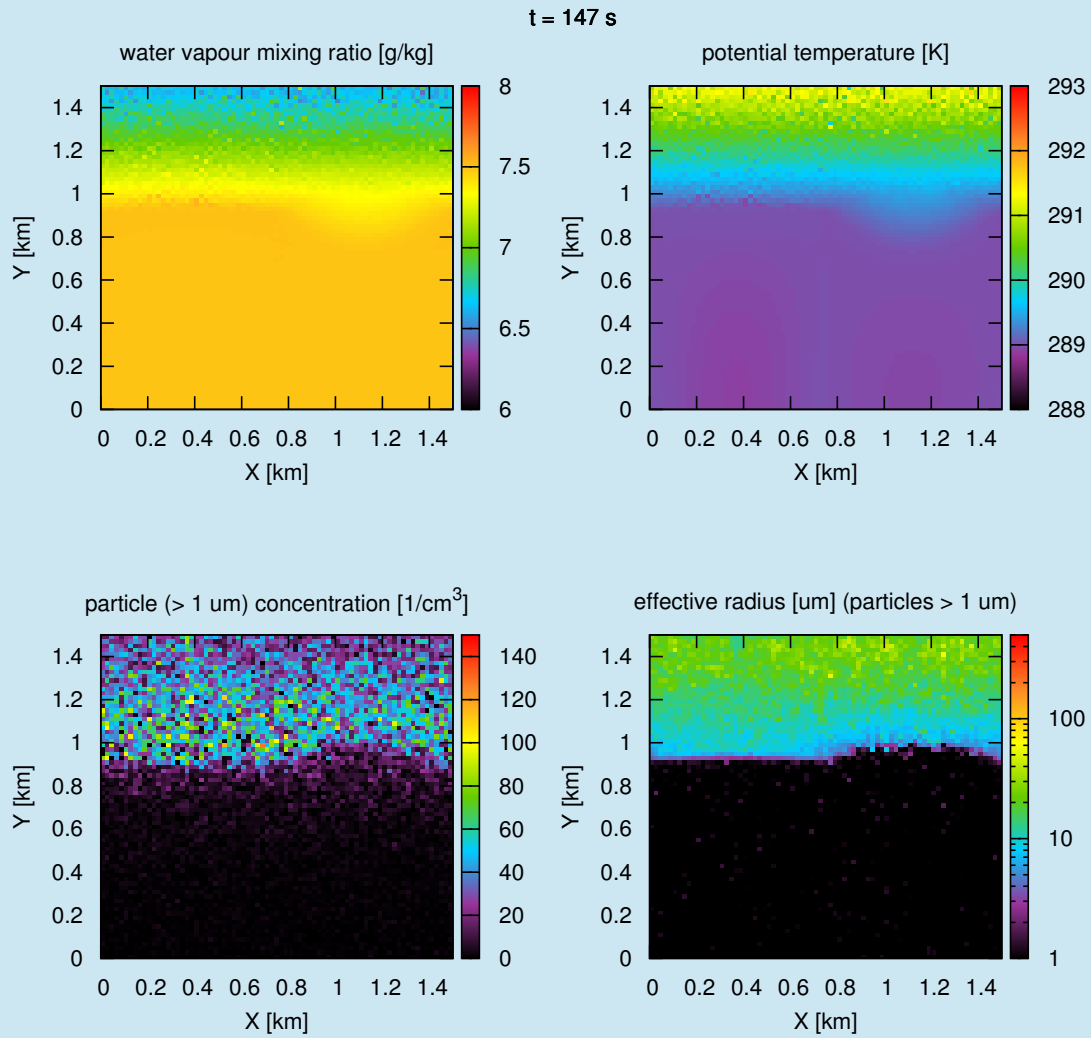

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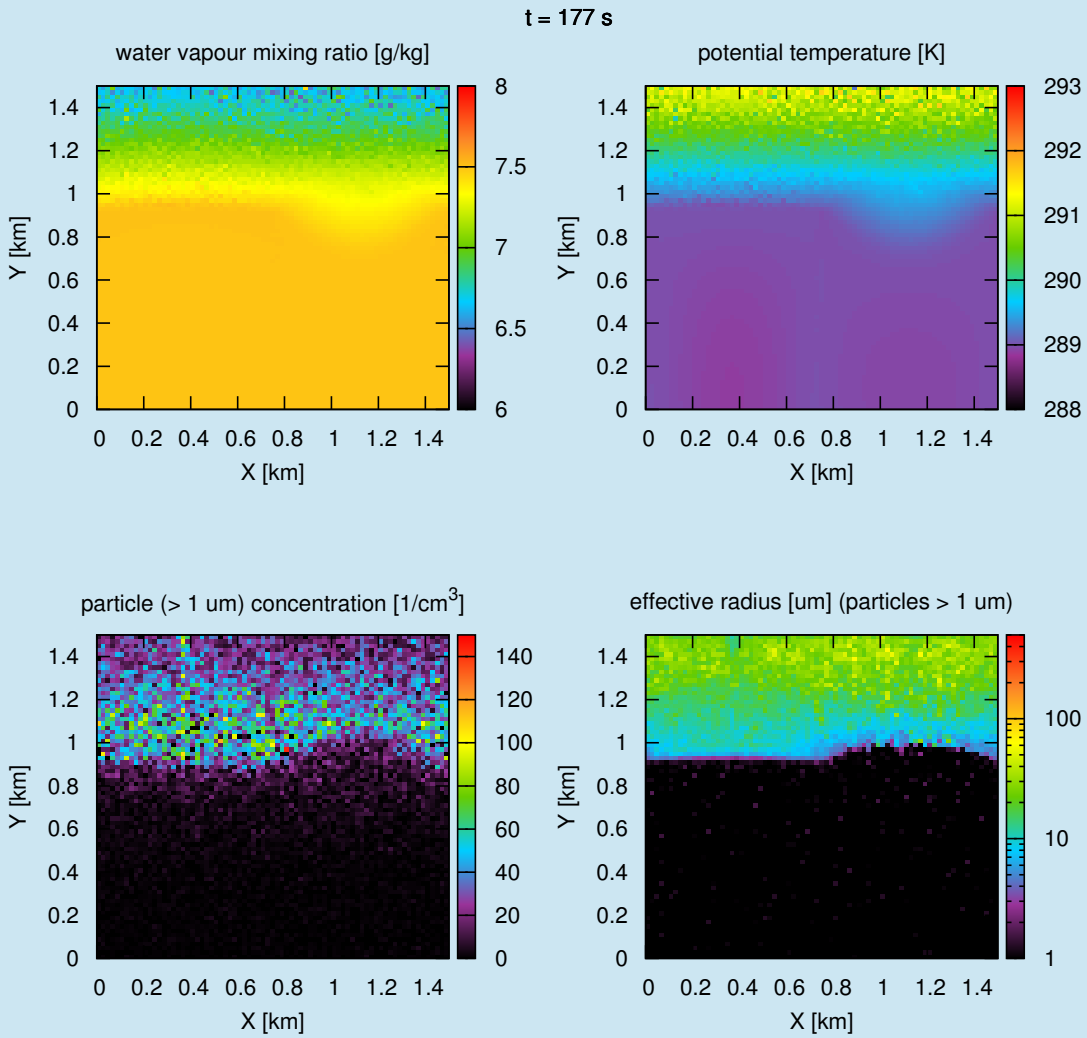

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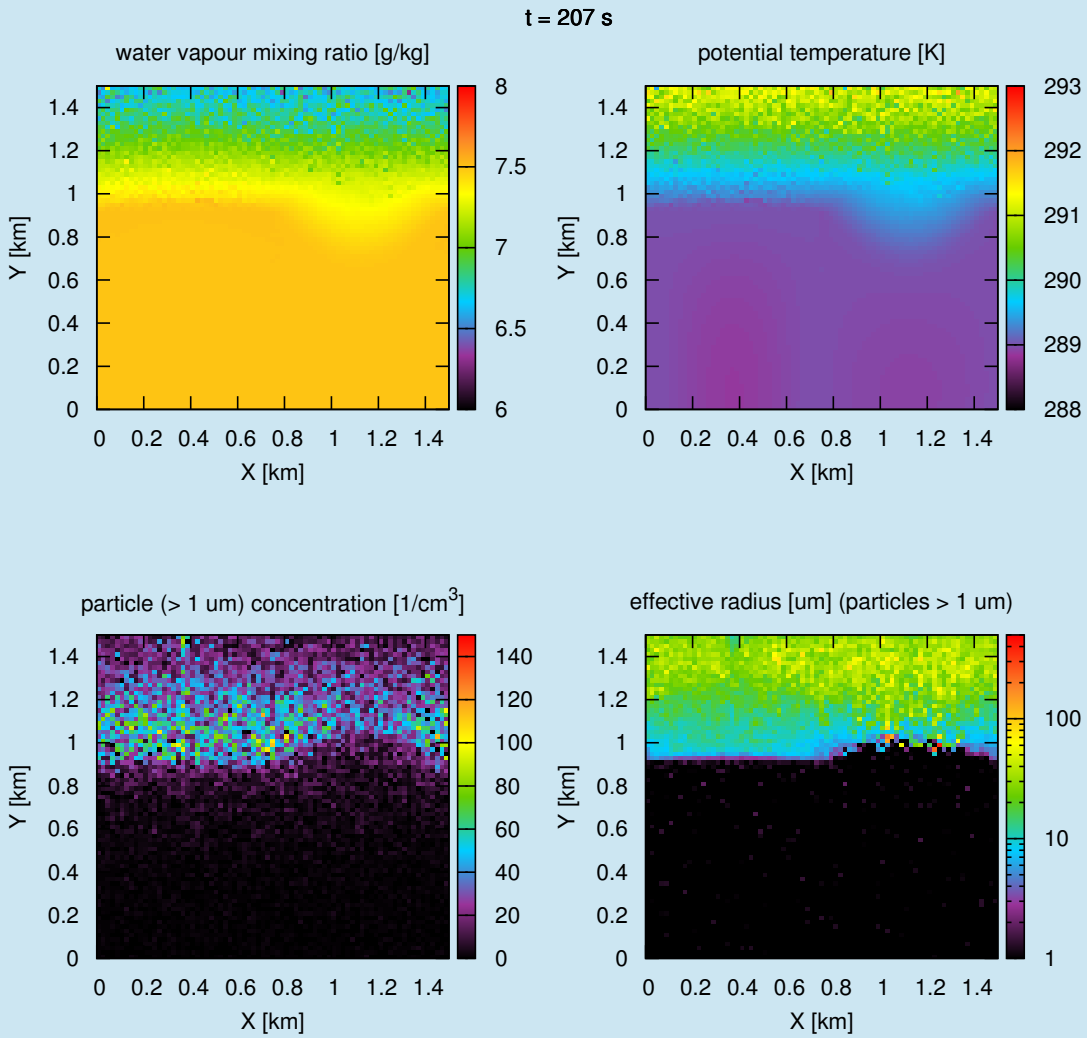

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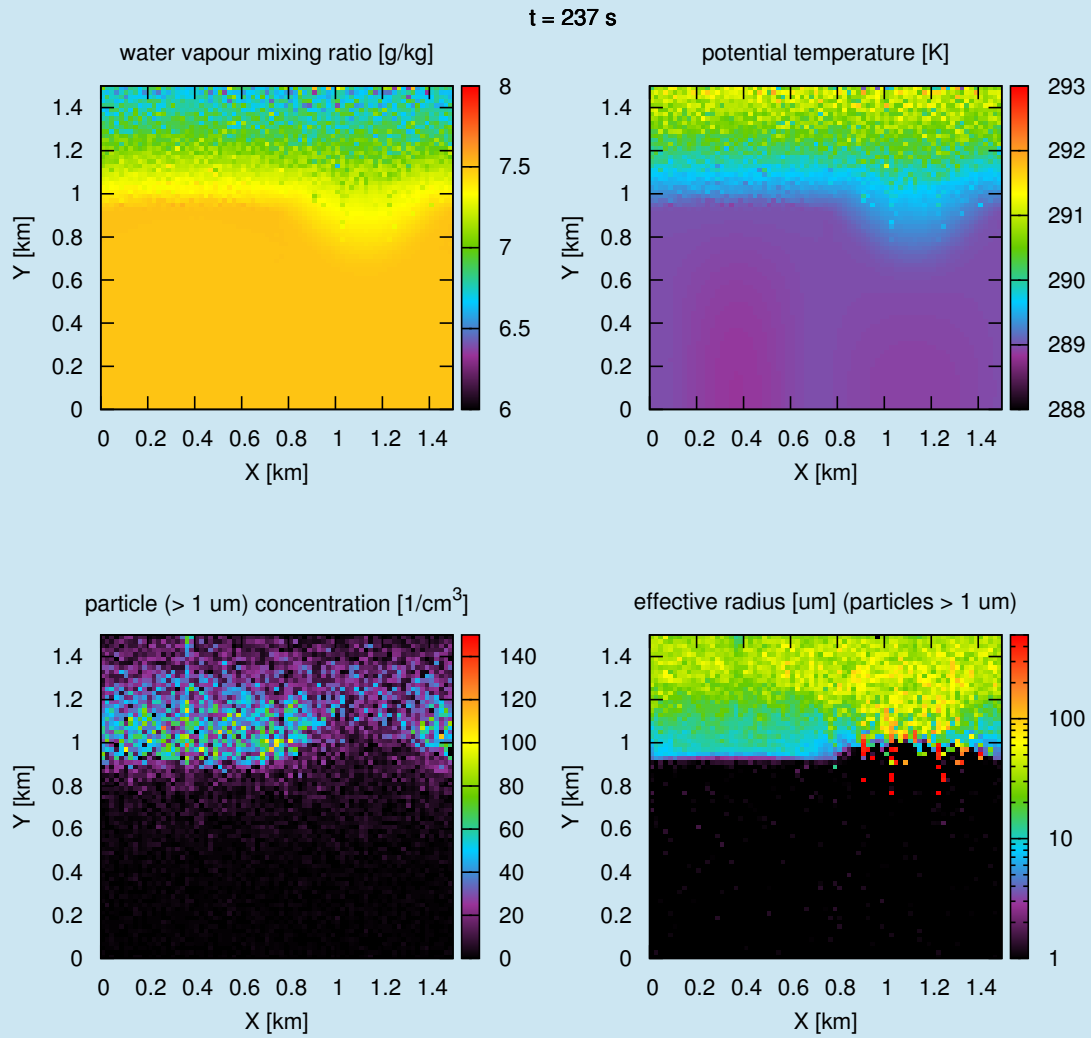

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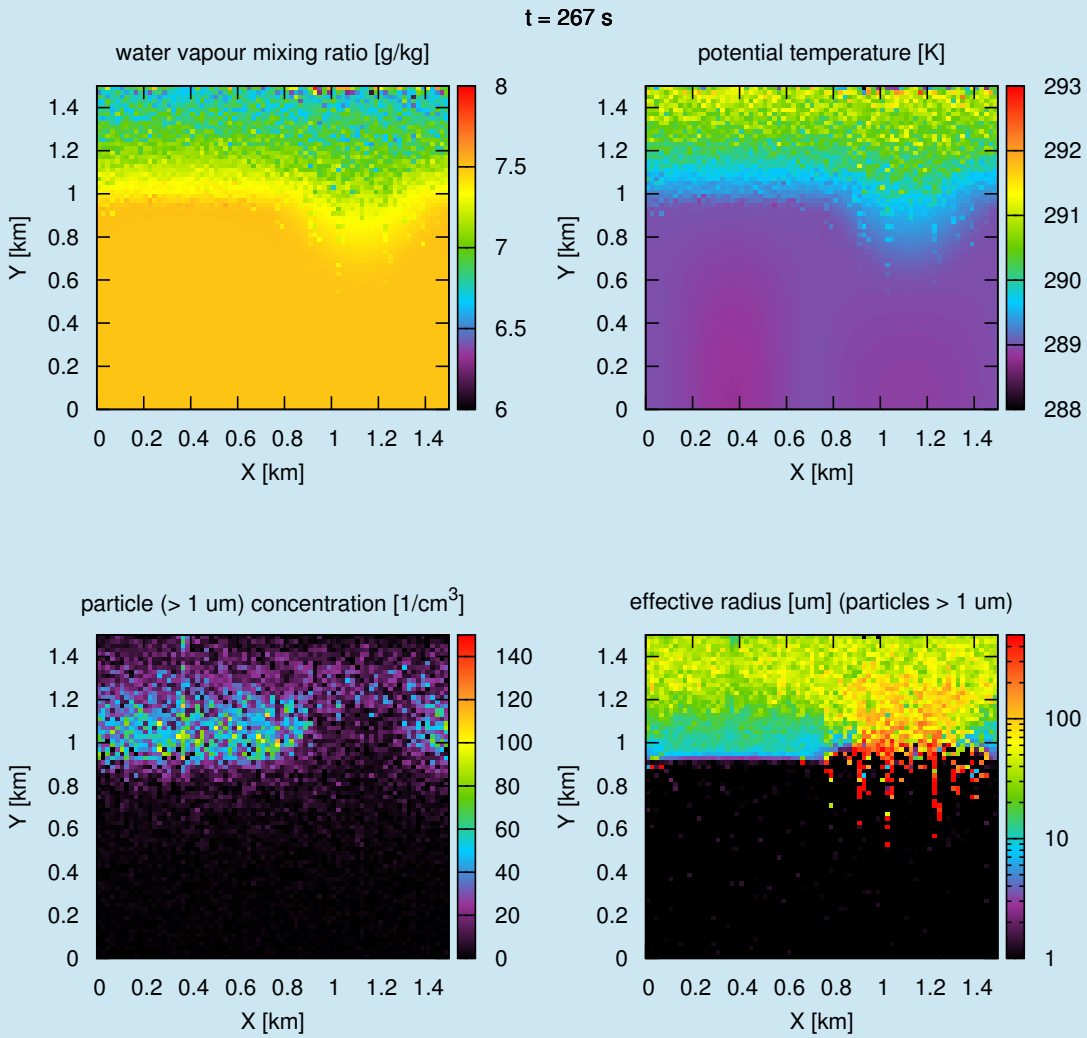

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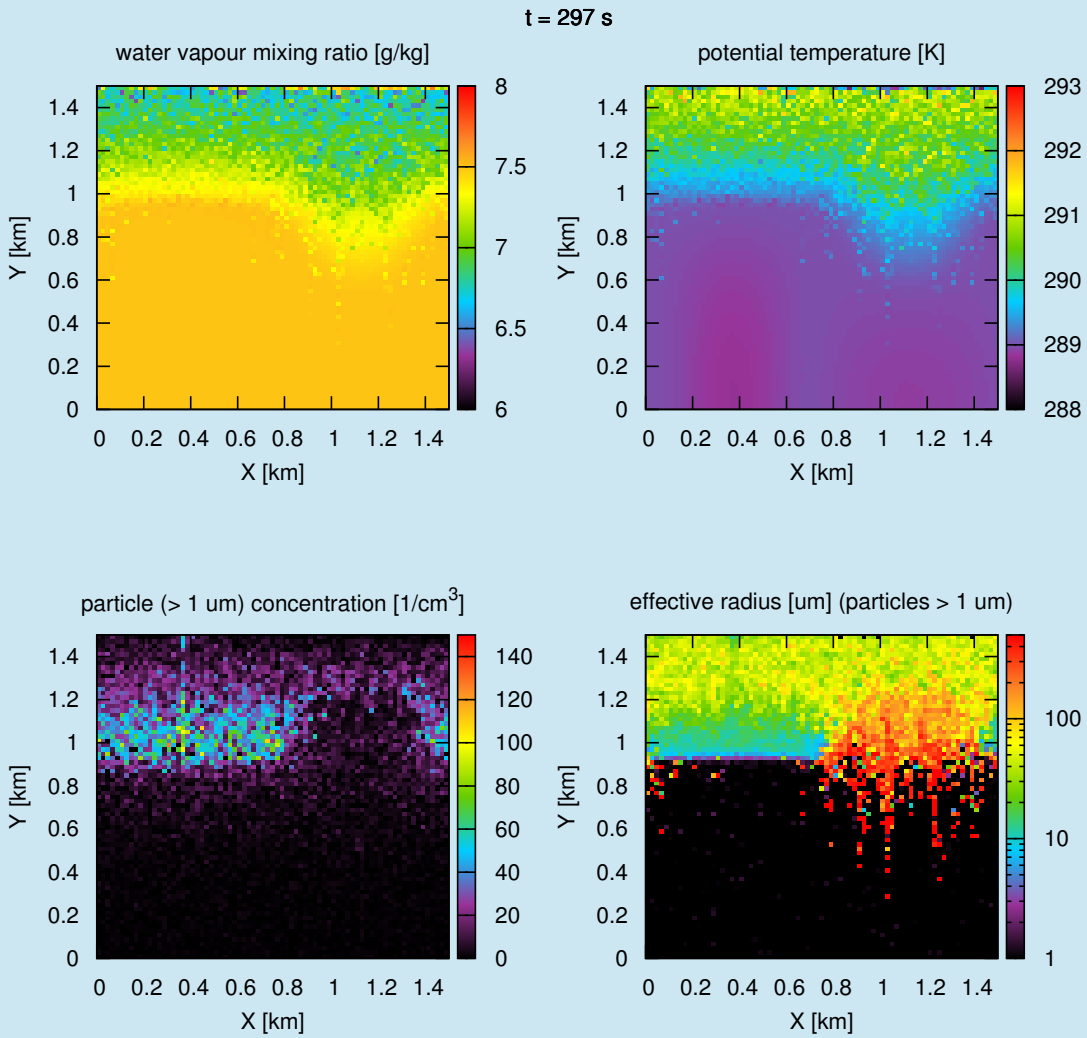

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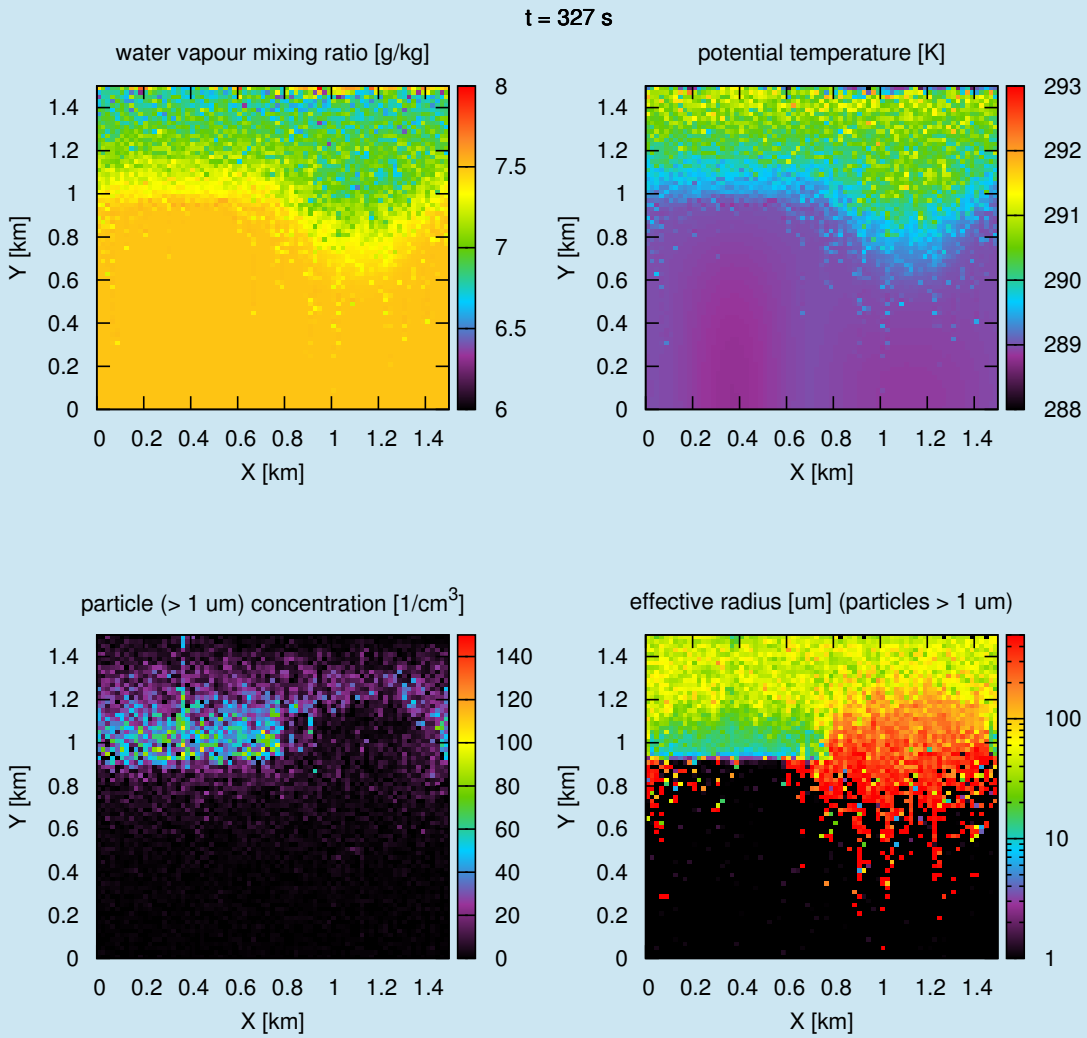

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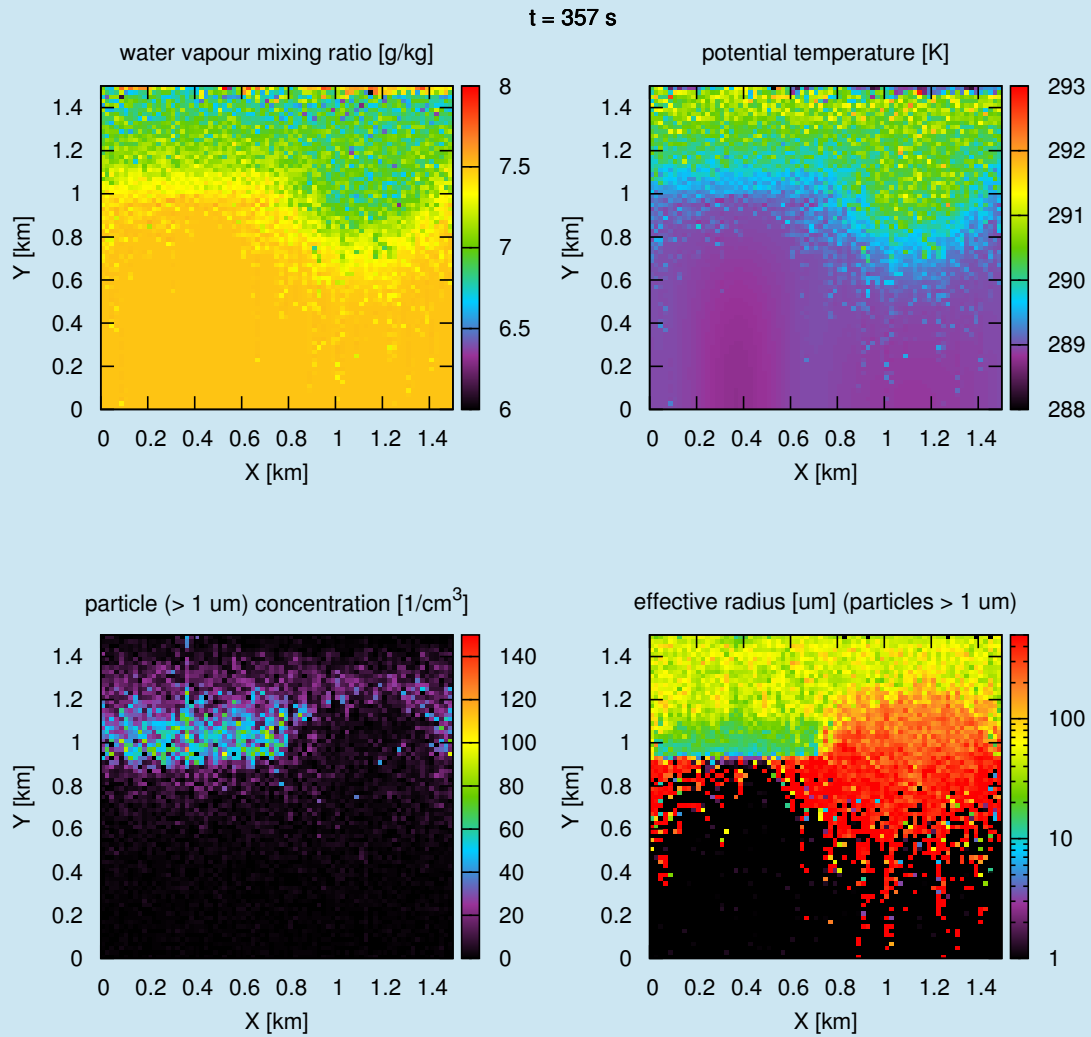

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icicle: currently available components

- advection scheme:
  - MPDATA
    - any number of iterations
    - 3rd order accuracy option
    - FCT (aka non-oscillatory) option
    - variable-sign field option
  - donor-cell, leapfrog, ...
- equation sets:
  - scalar advection (rhs=0 $\rightsquigarrow$ tests)
  - 1D/2D shallow water
  - 2D/3D isentropic
  - 2D moist kinematic (this workshop's "case 1")
    - bulk (Kessler) μ-physics
    - particle-based (super-droplet) μ-physics
- input/output: ASCII, netCDF-4
- ...

all selectable at runtime via command-line options

$\rightsquigarrow$ command-line string unambiguously defines simulation (in output file)

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- and:
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beta planned for 2013 Q2 (code & docs)

Thanks for your attention!

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Merali 2010 (Nature, vol. 467, p. 775-777)

http://www.nature.com/news/2010/101013/full/467775a.html

return_macro() definition (preprocessor)

```
#define return_macro(expr) \
  -> decltype(safeToReturn(expr)) \
  { return safeToReturn(expr); }
```