Object-oriented numerics in C++, Python and modern Fortran

a case study comparison

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Maciej Fijałkowski

PyPy Team

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Boulder, 2nd April 2013

background

Object oriented programming (OOP) *"has become recognised as the almost unique successful paradigm for creating complex software"*

Press et al. 2007: Numerical Recipes – The Art of Scientific Computing

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Application of OOP for numerical modelling software may help to:

- maintain modularity and separation of program logic layers (e.g. separation of numerical algorithms, parallelisation mechanisms, data input/output, error handling and the description of physical processes); and

- **shorten and simplify the source code by reproducing the mathematical notation used in the literature**.

both contribute to software maintainability and auditability

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we need software maintainability and auditability!

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

(climate modelling context)

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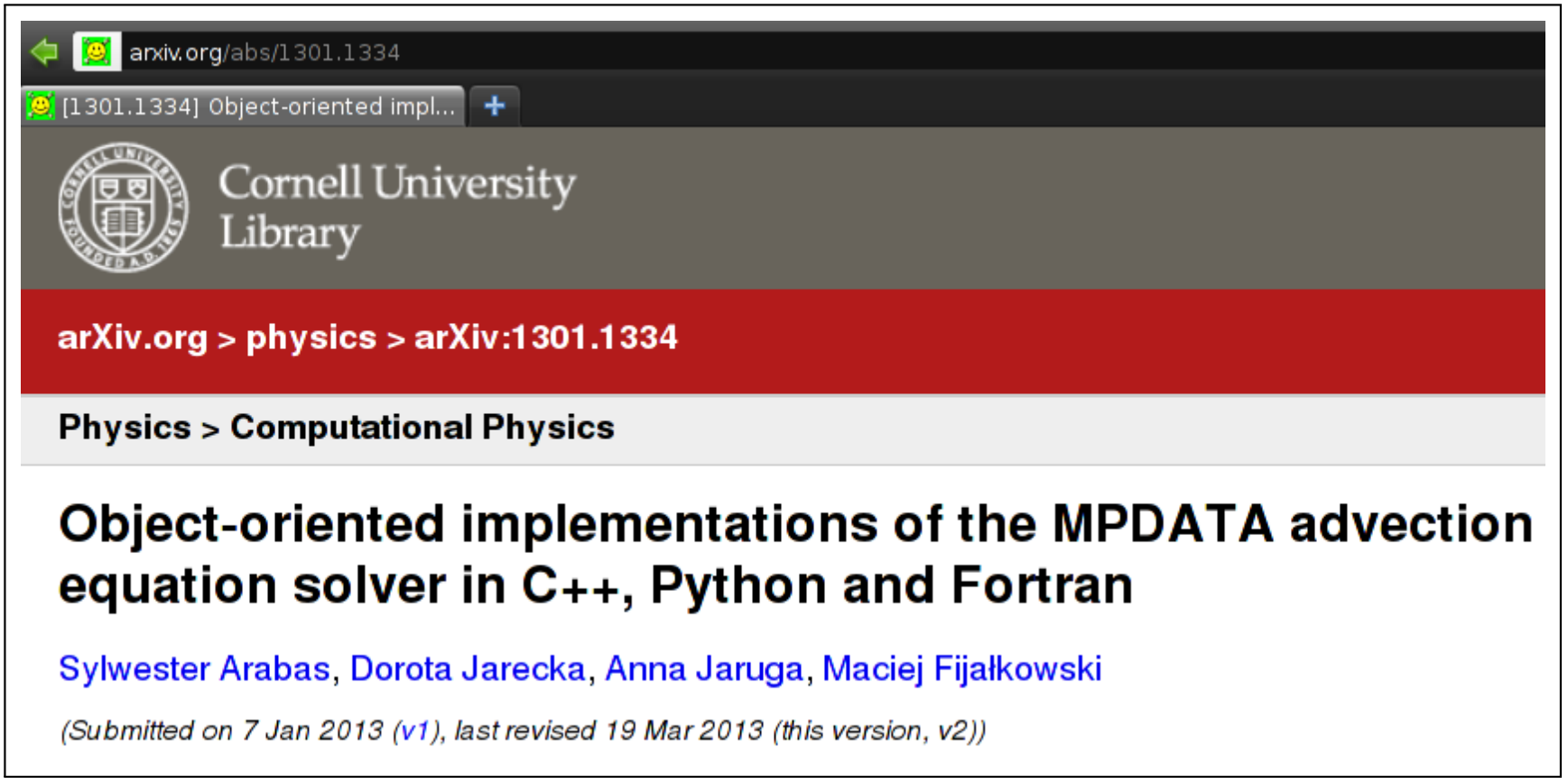

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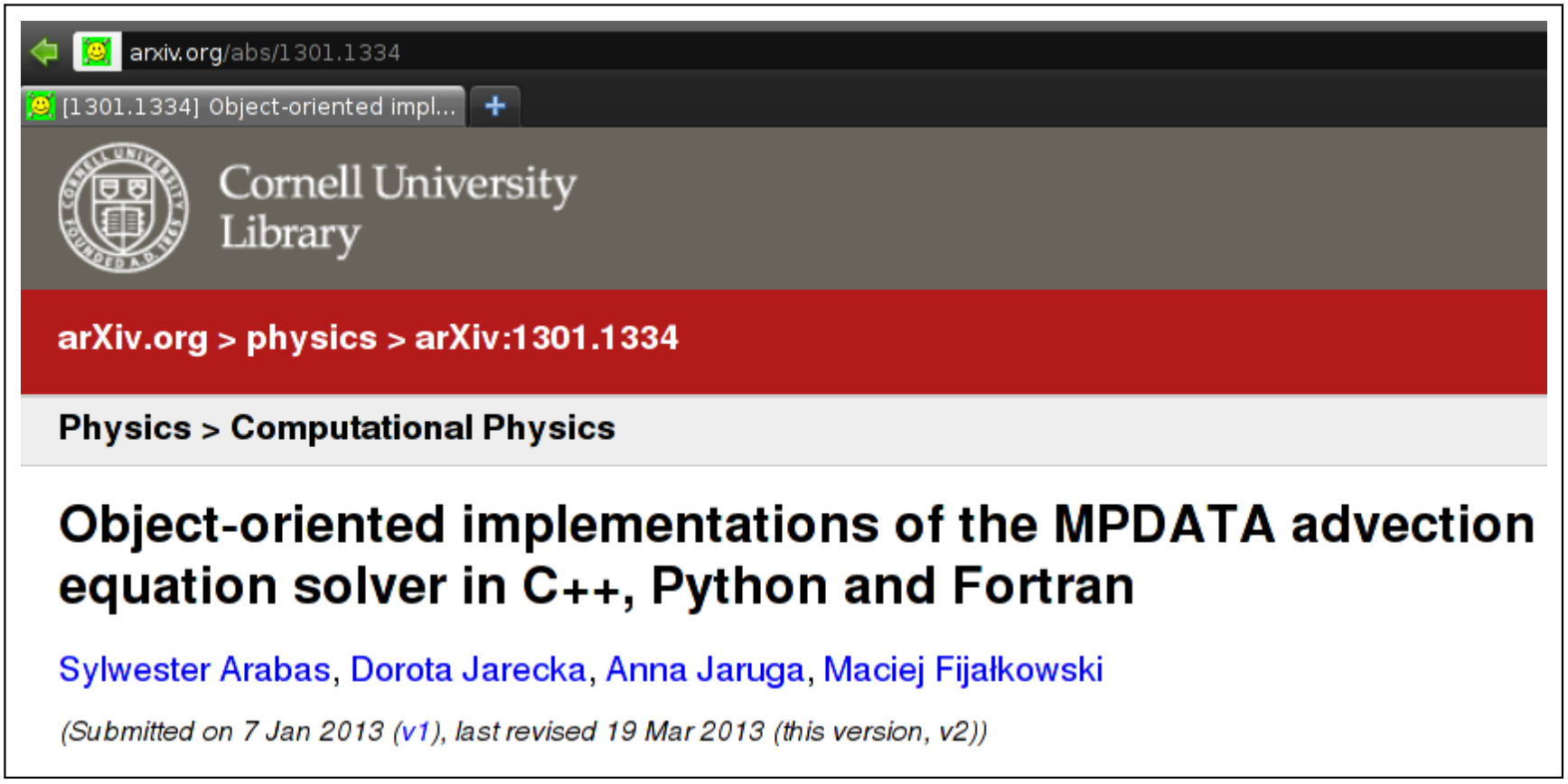
  - take an algorithm used in the cores of weather/climate models
  - implement it using OOP in C++, Python and Fortran
  - discuss **all** the code (inlined in the paper text)
  - compare language/library features and performance
- submitted to Comp. Phys. Comm.
- code: github.com/slayoo/mpdata/



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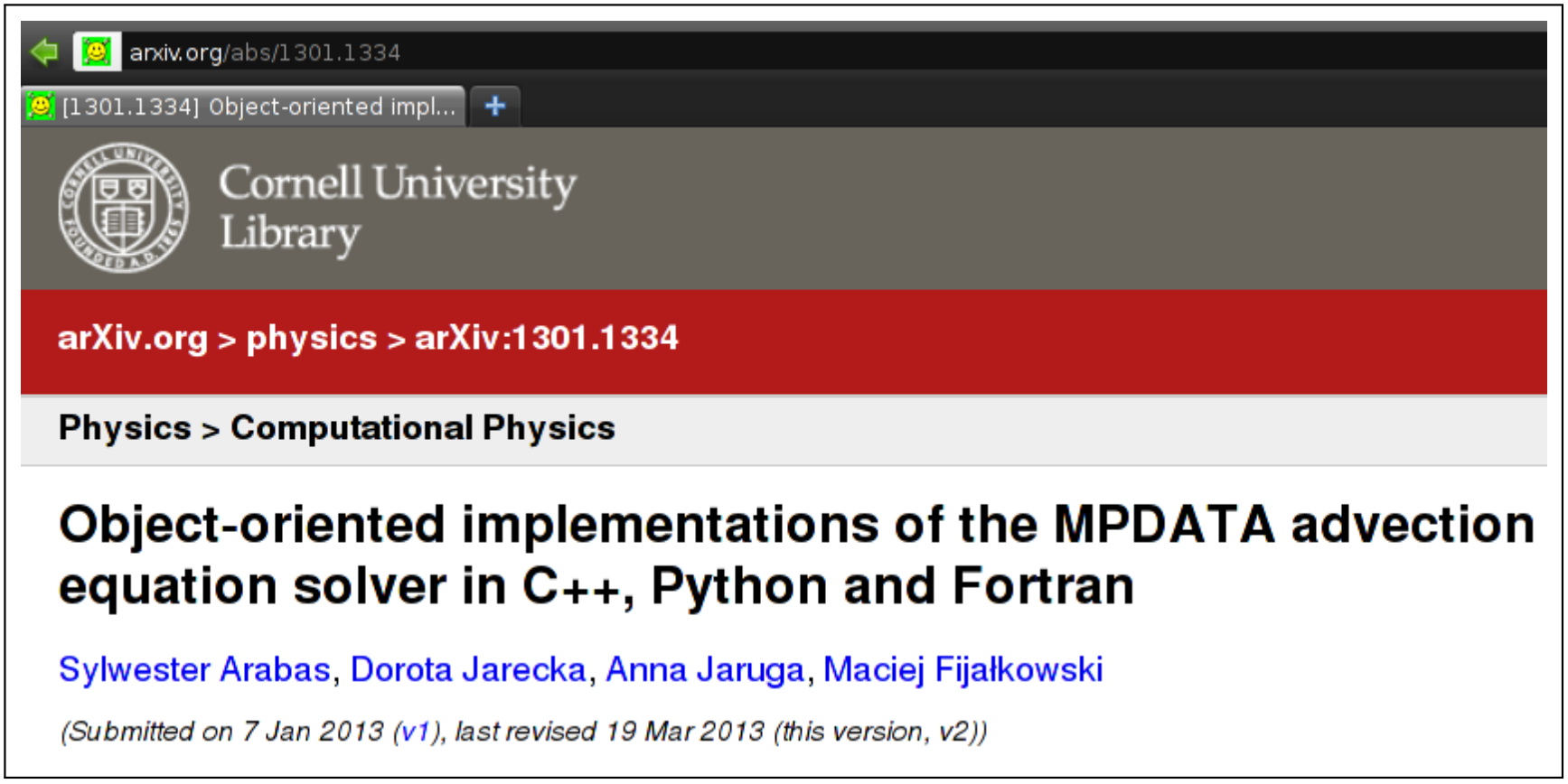

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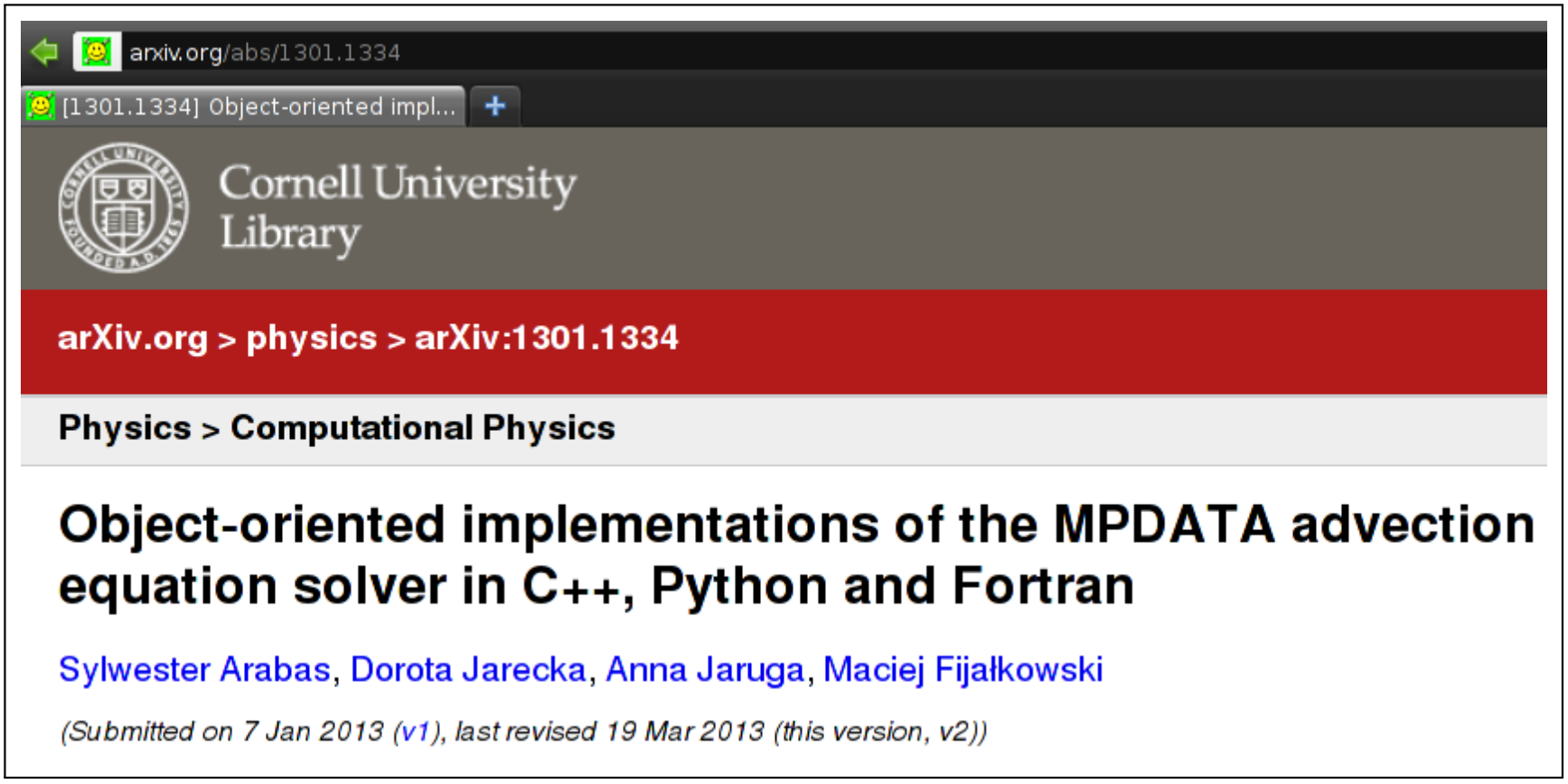

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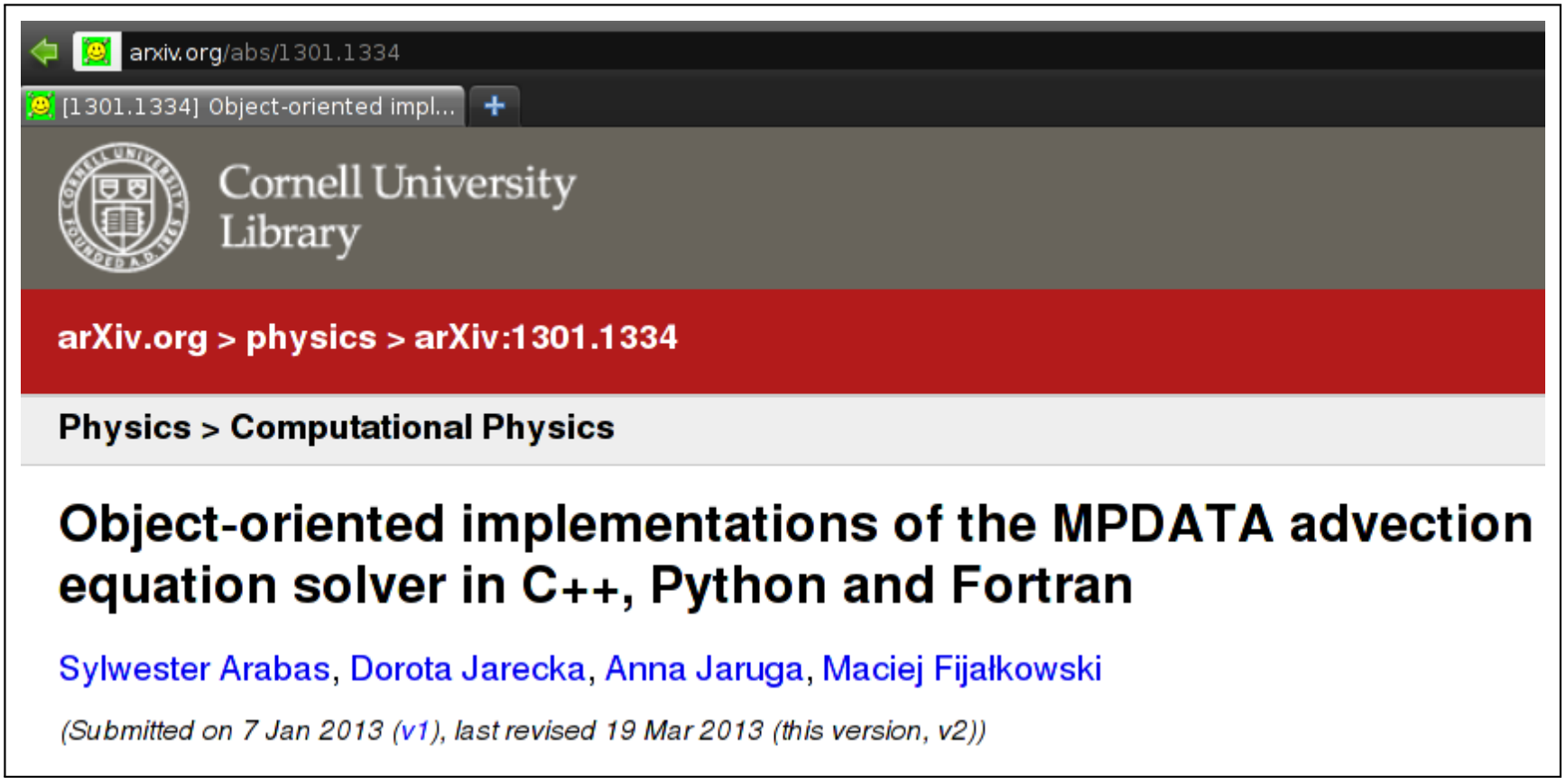

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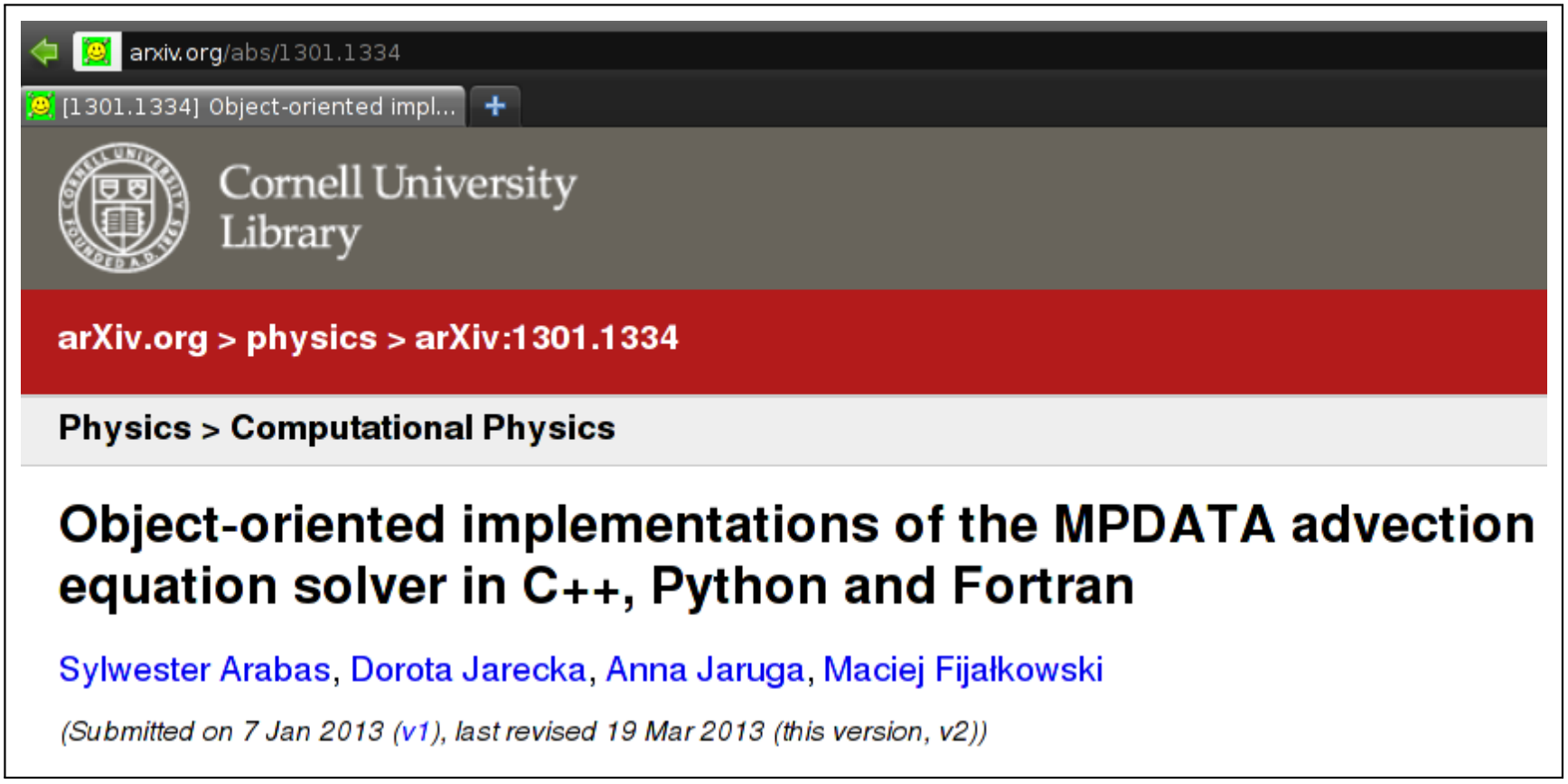

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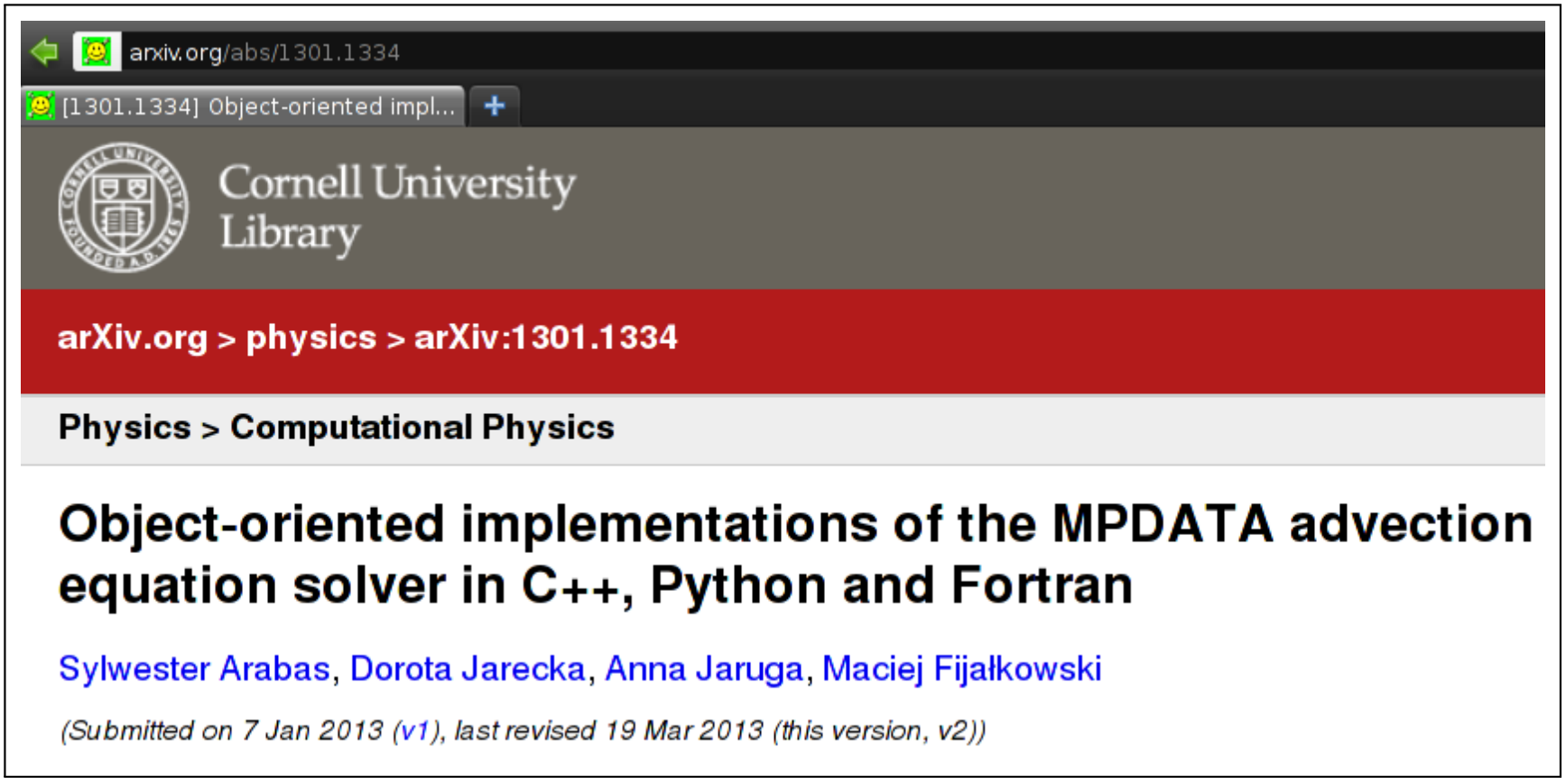

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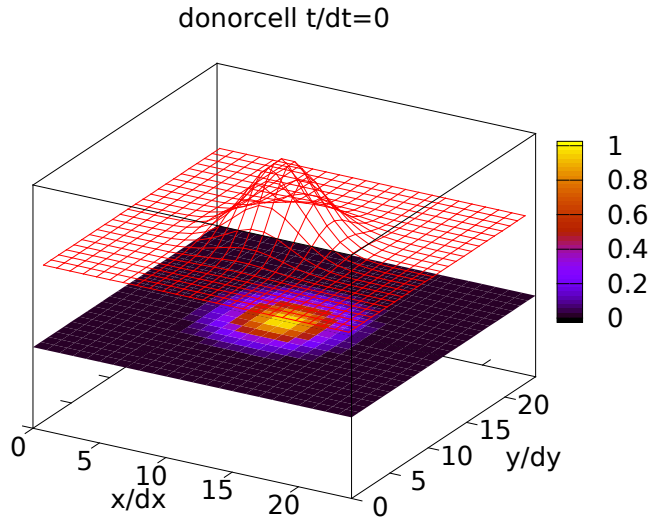
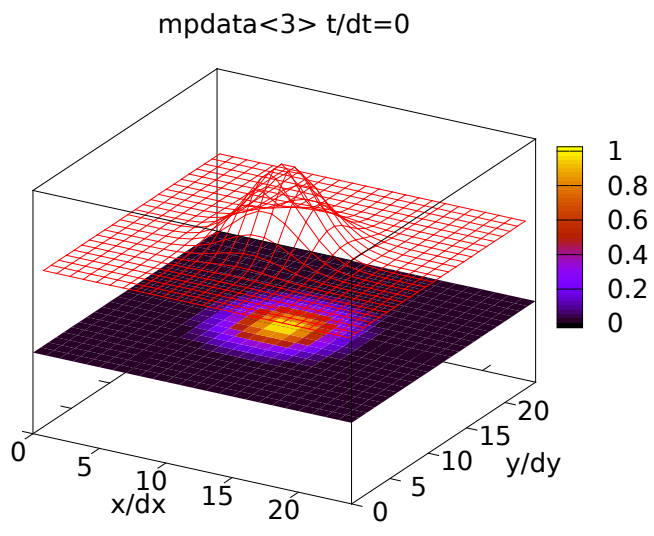
plan of this talk

- background
- MPDATA in pictures & formulæ
- MPDATA in C++, Python & Fortran
  - highlights from three OOP implementations
  - performance evaluation
- language choice tradeoffs
- future plans and a take-home message

MPDATA (Smolarkiewicz 1984) in pictures





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- non-oscillatory (optionally)
- multi-dimensional & sign-preserving by design
- readily parallelisable
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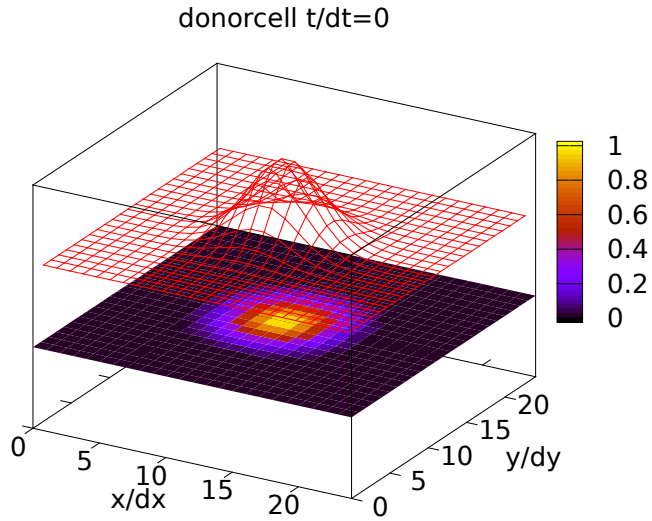

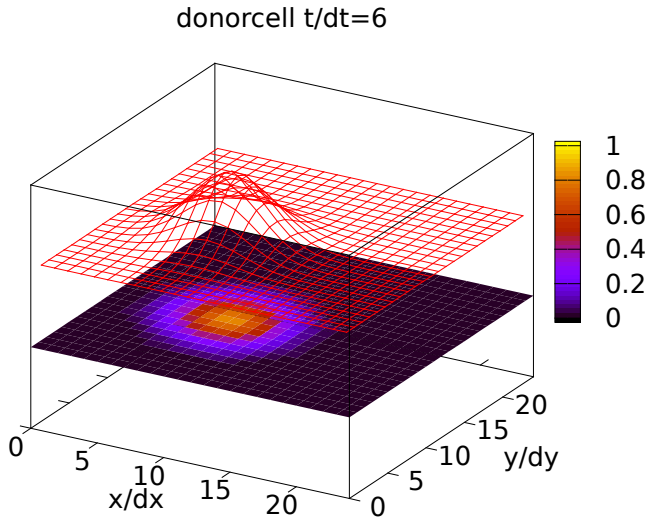

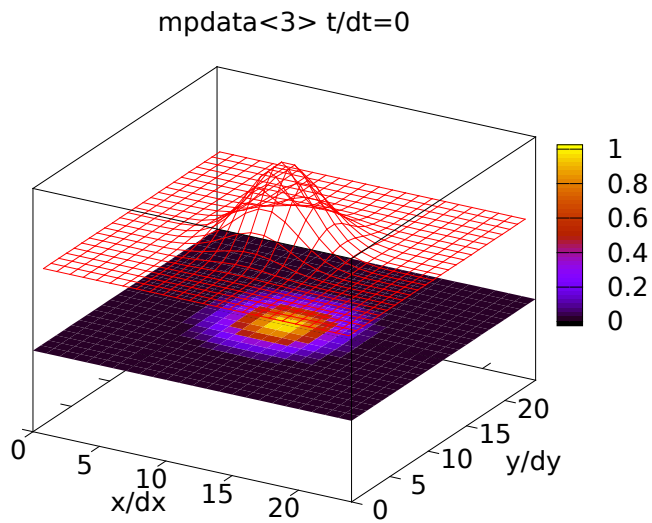

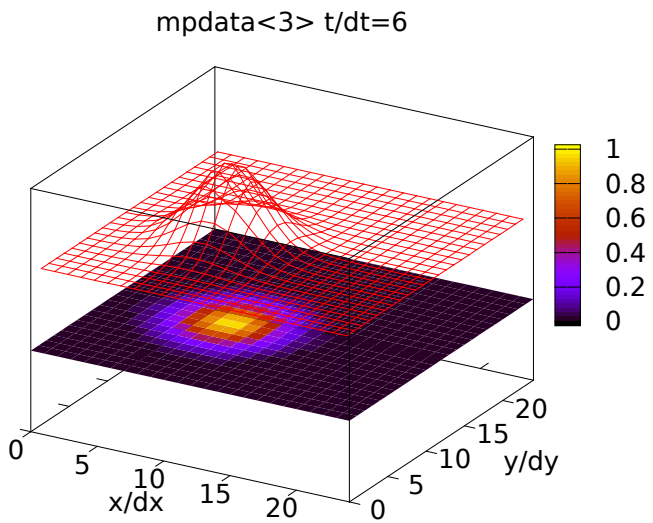

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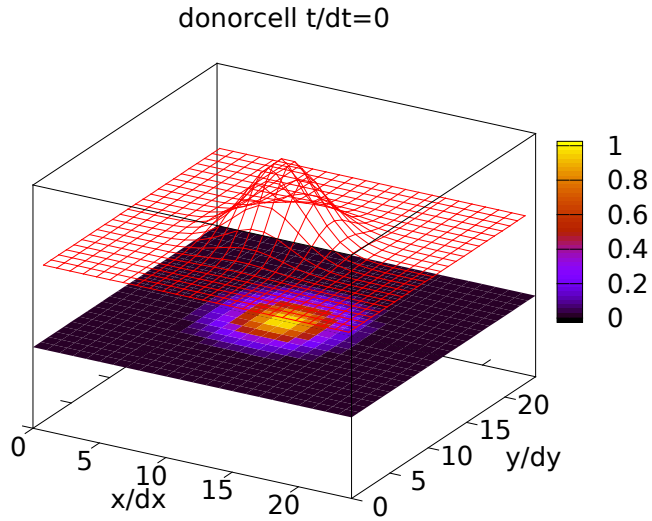

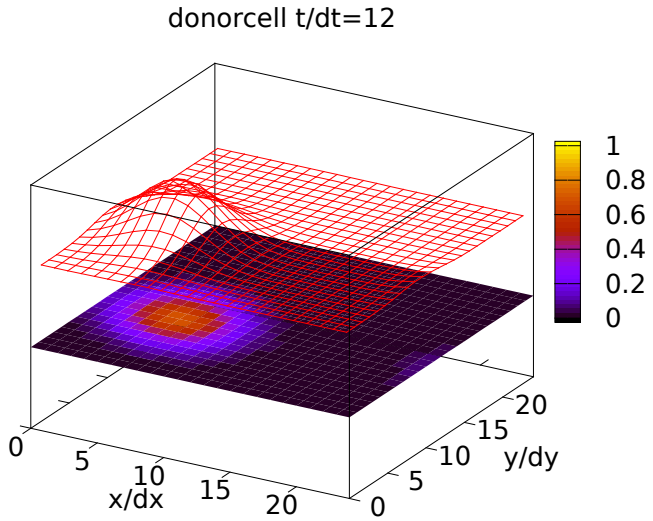

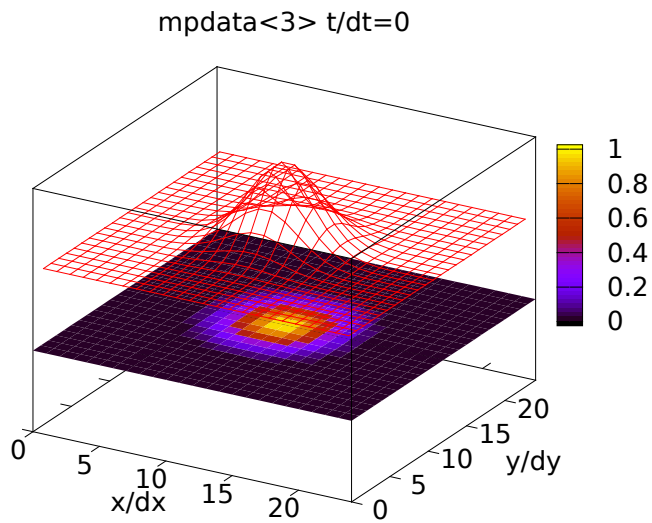

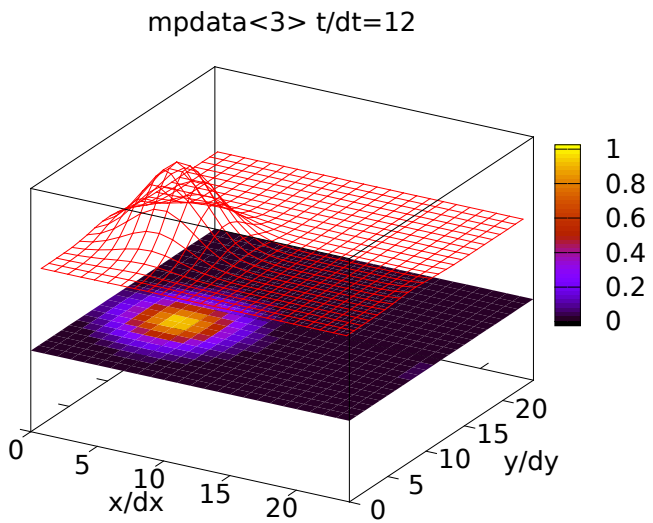

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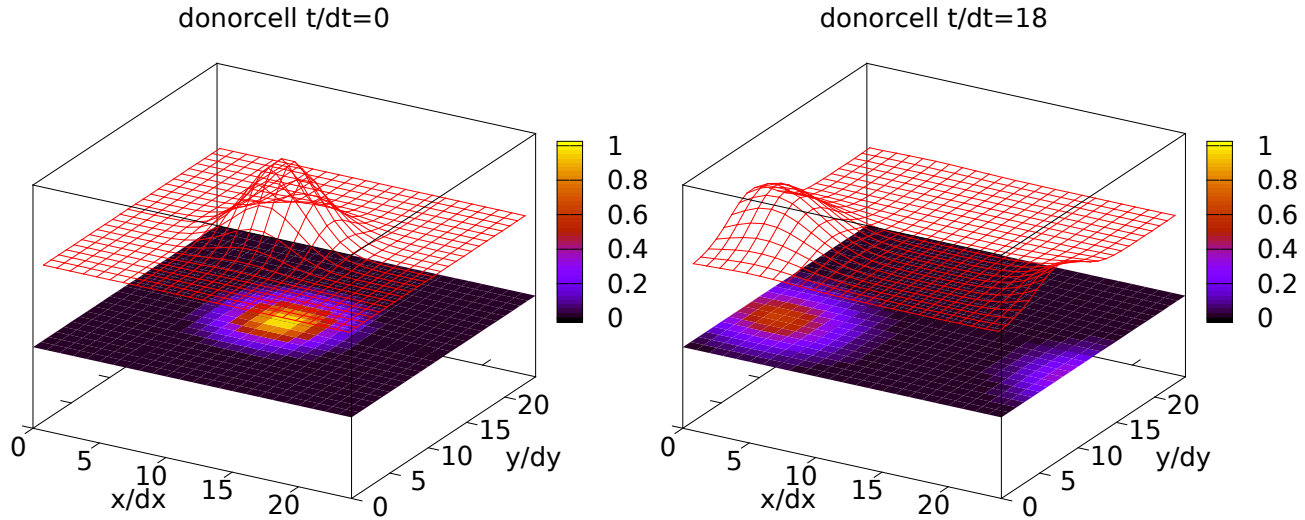

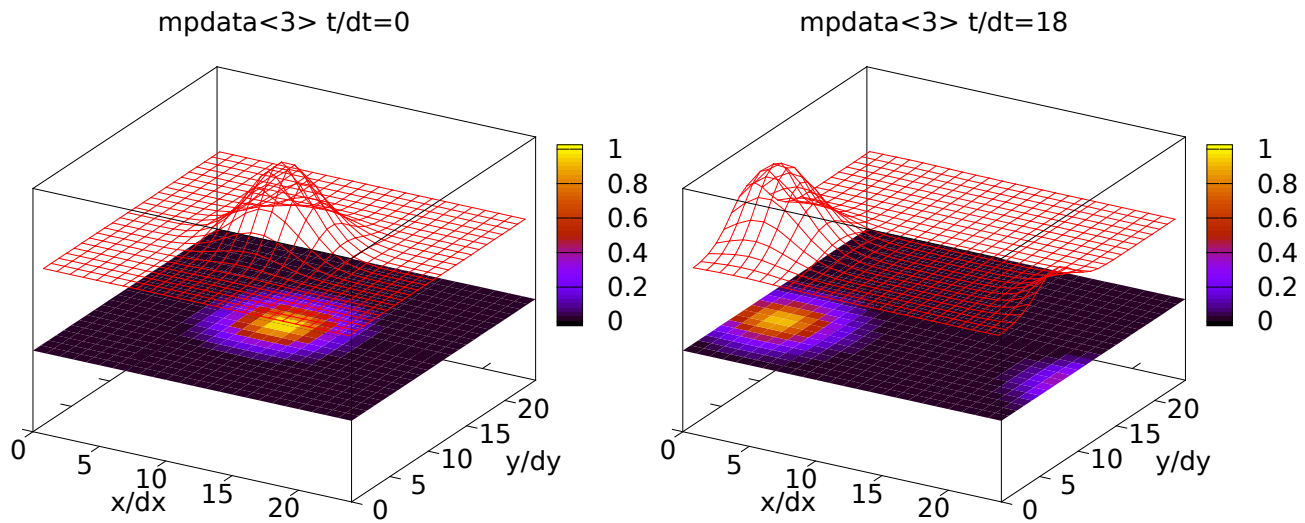

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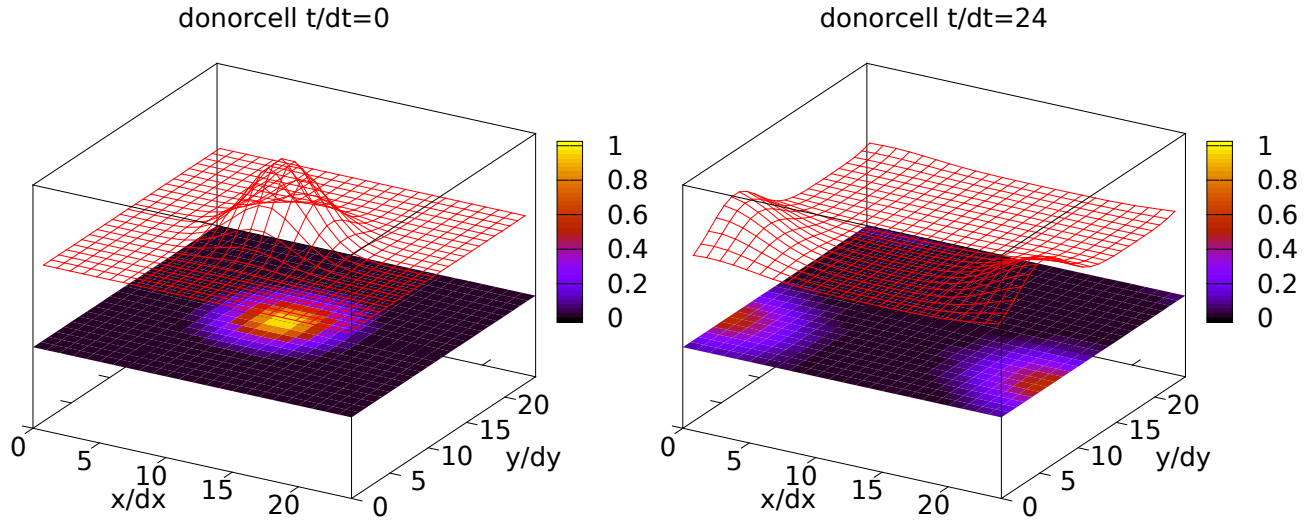

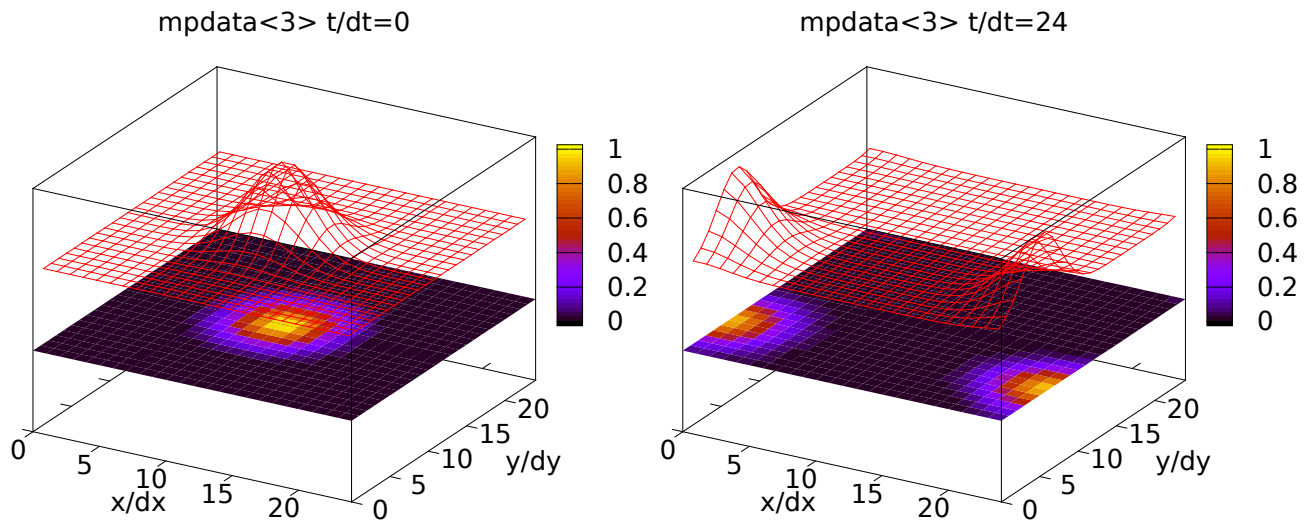

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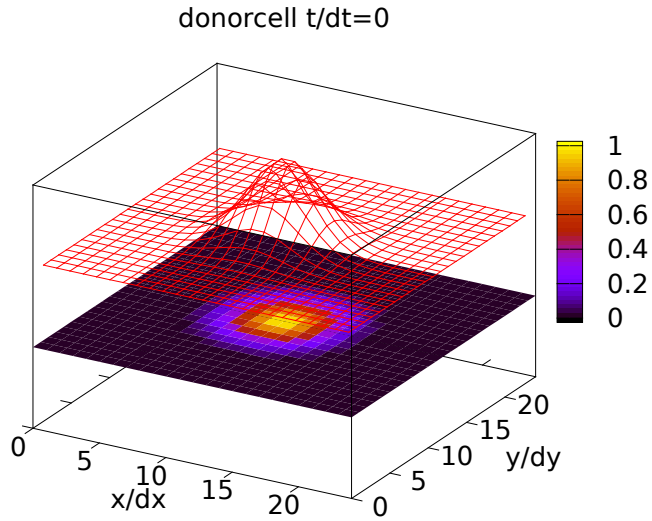

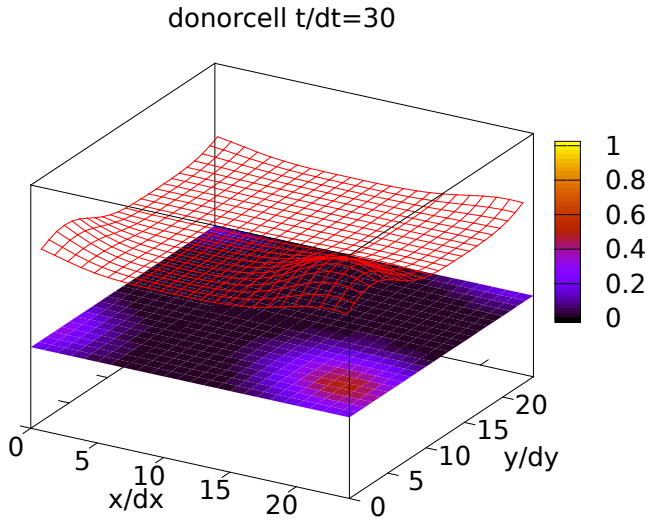

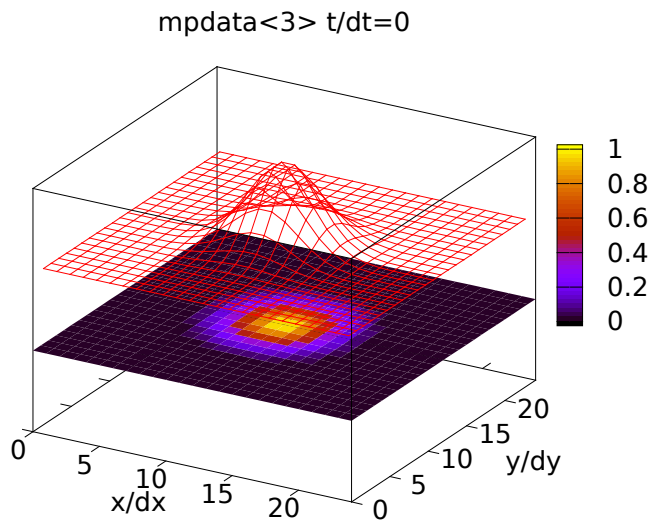

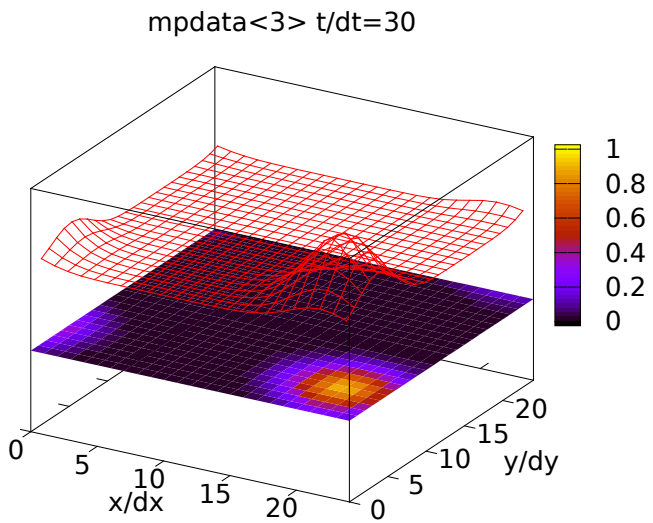

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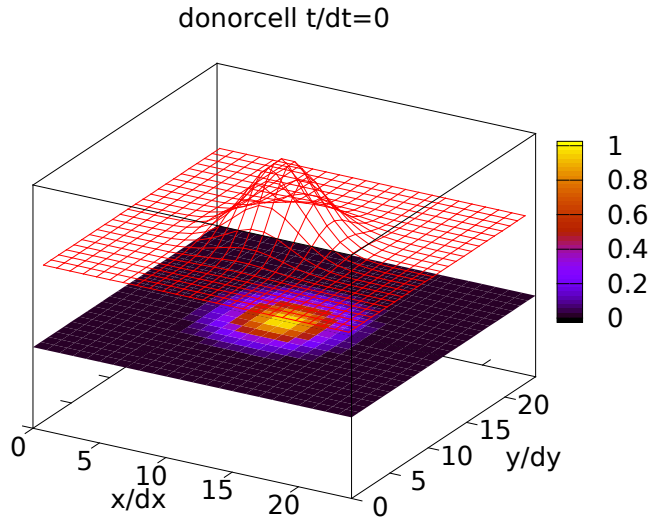

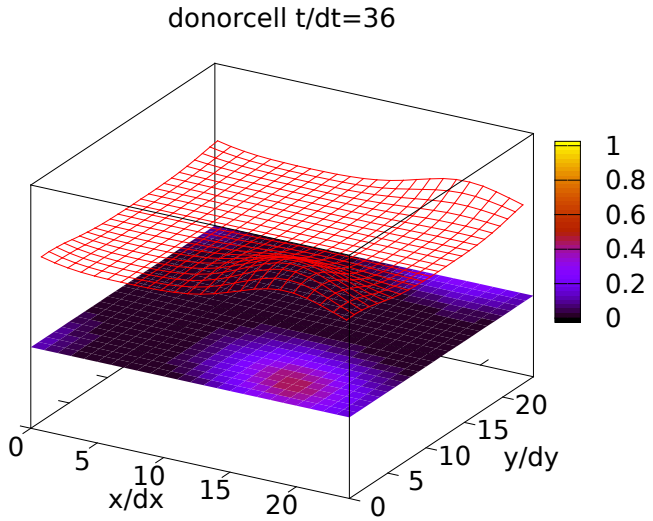

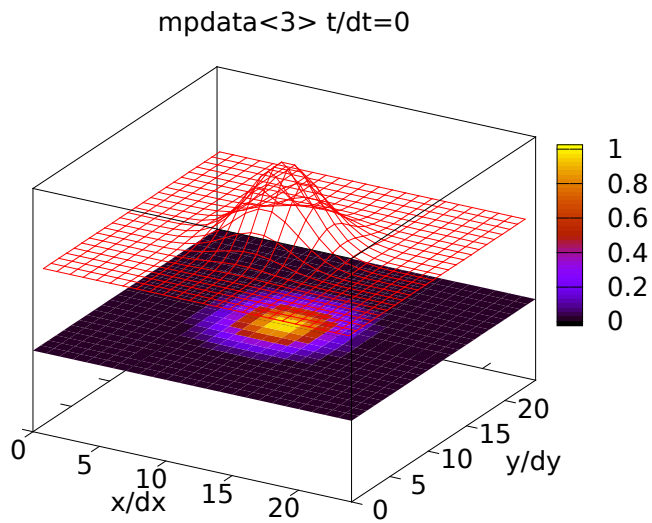

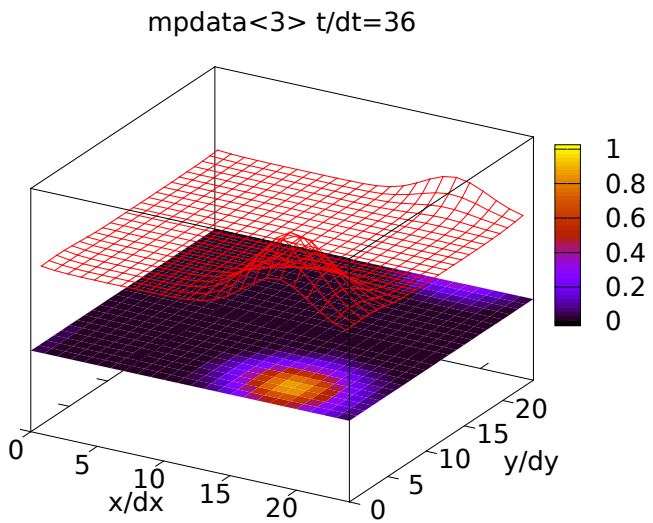

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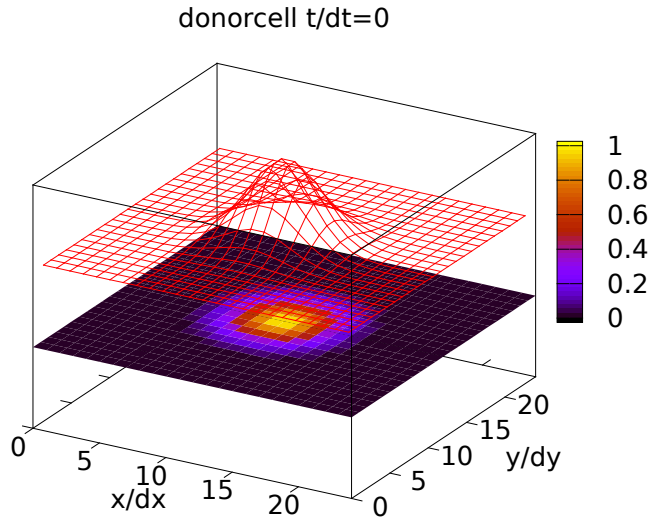

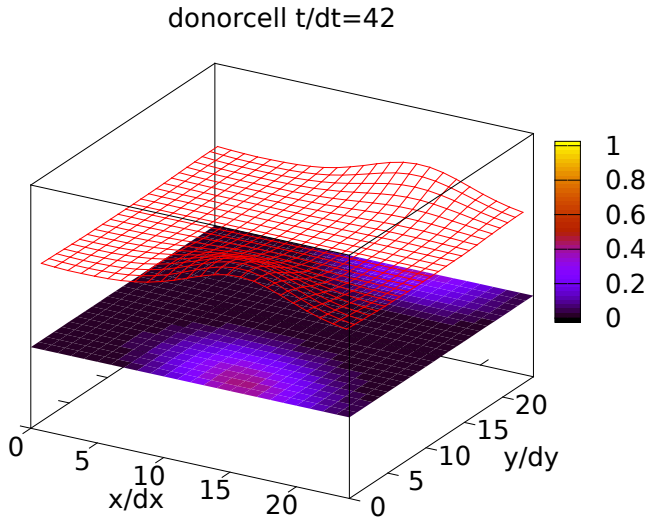

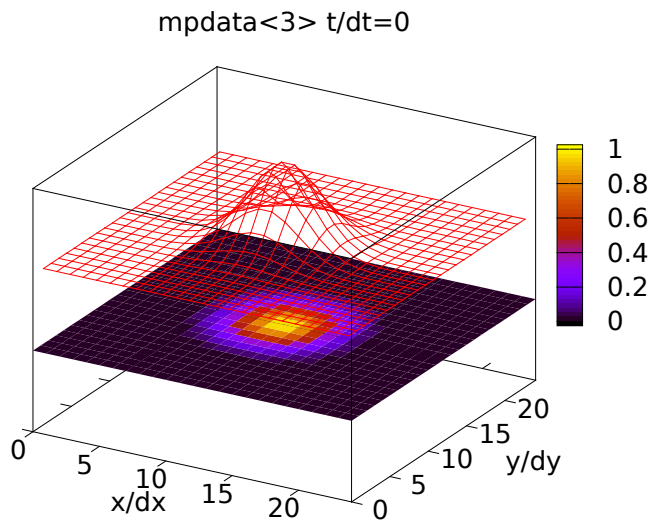

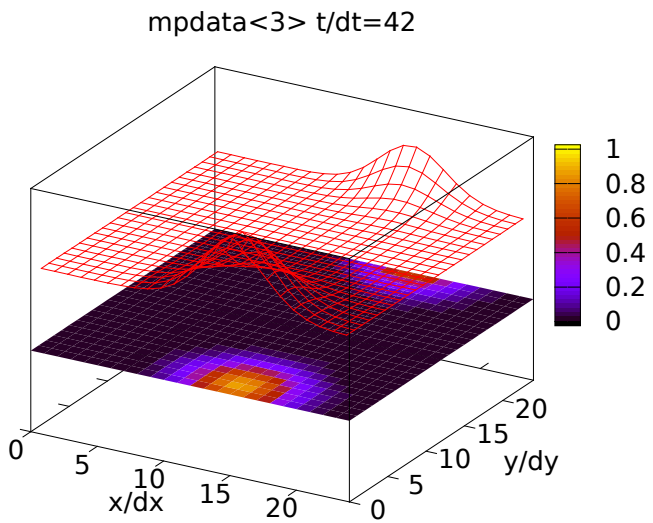

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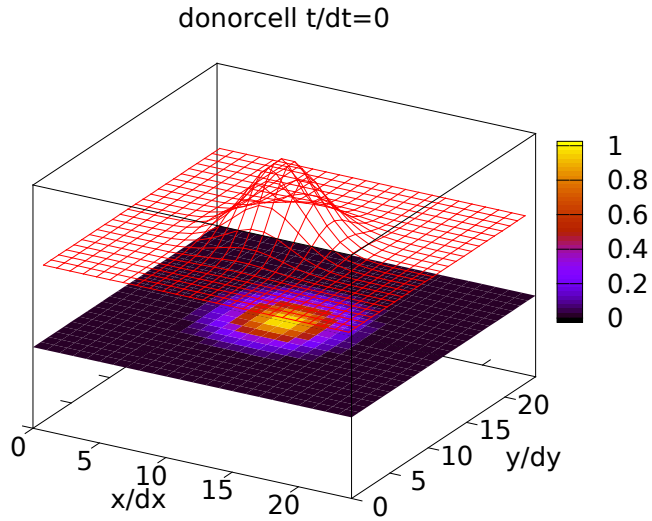

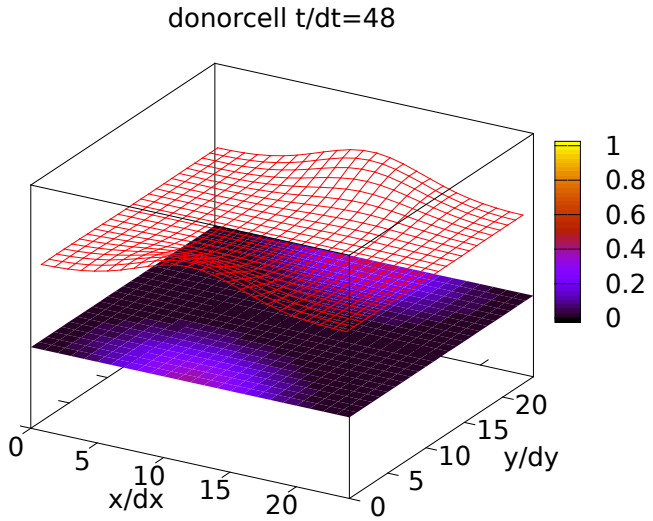

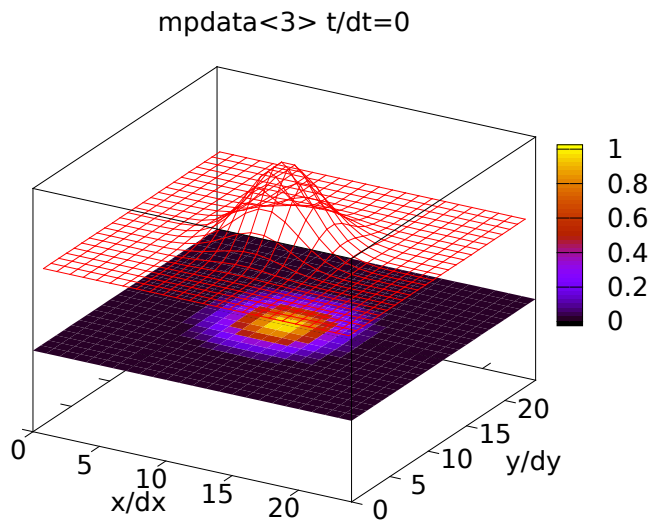

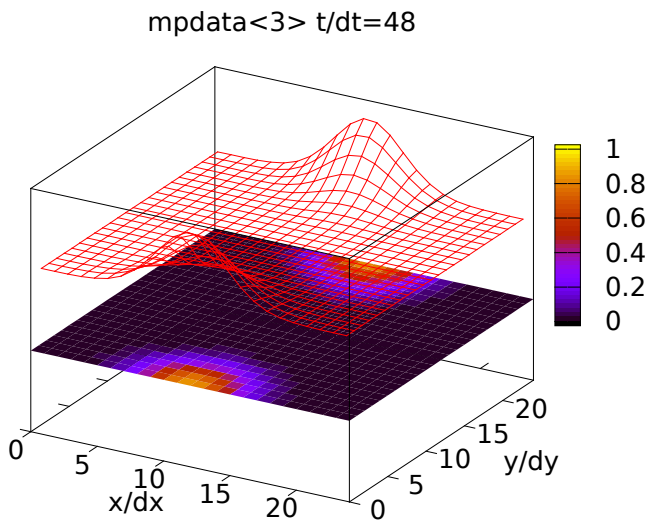

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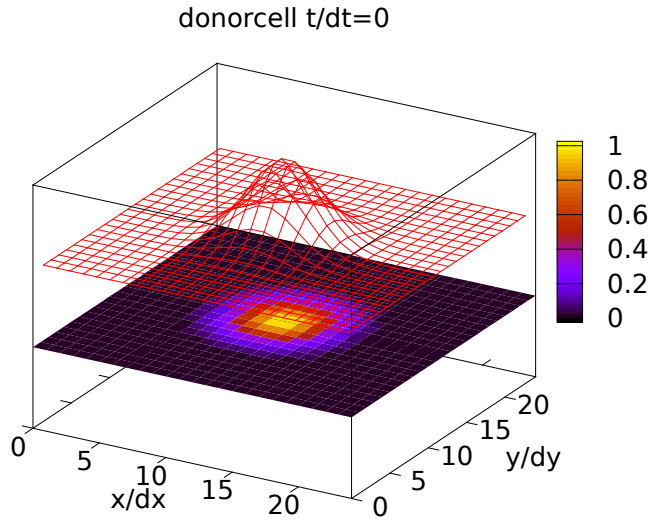

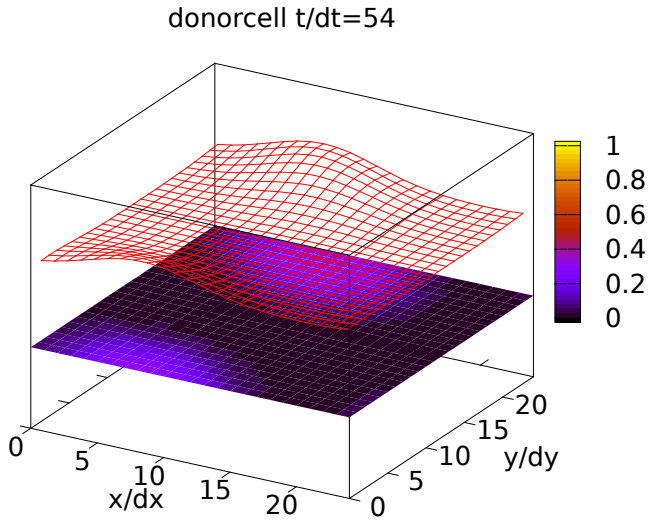

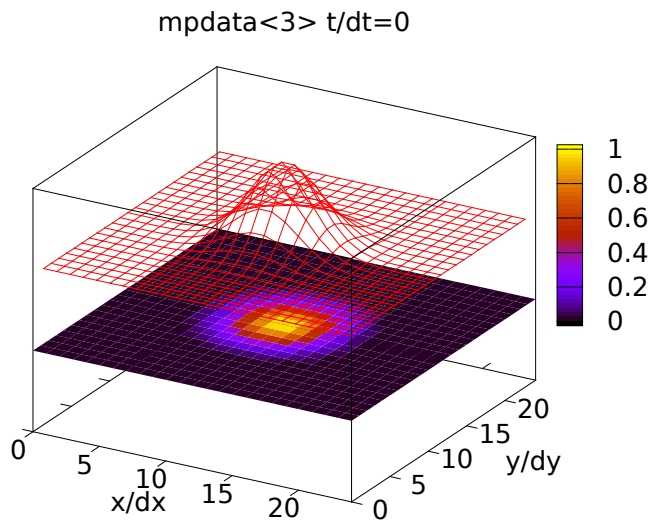

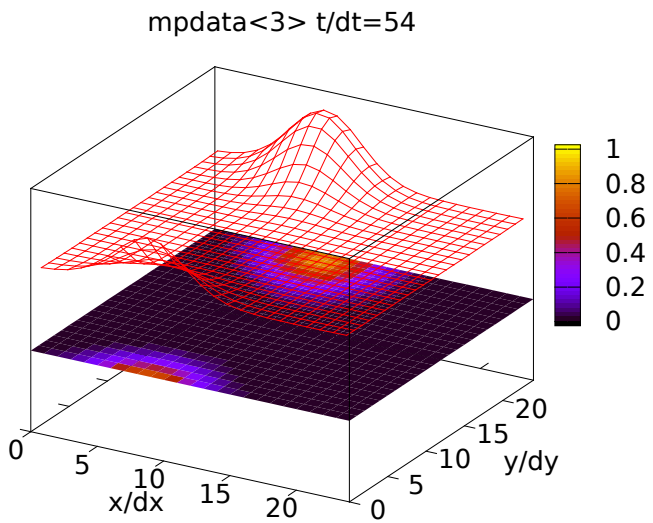

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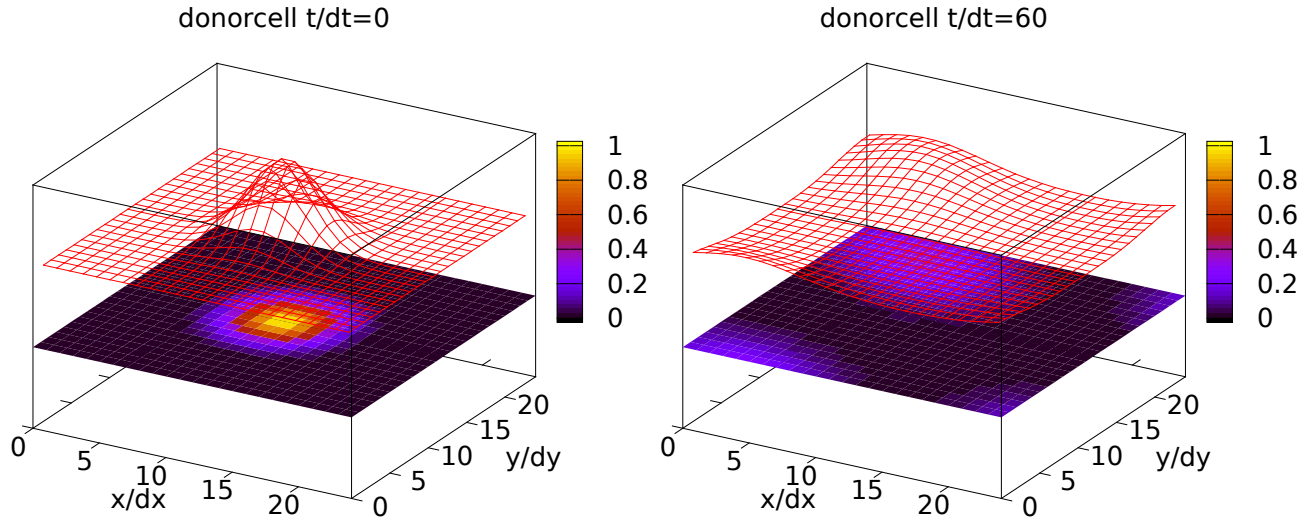

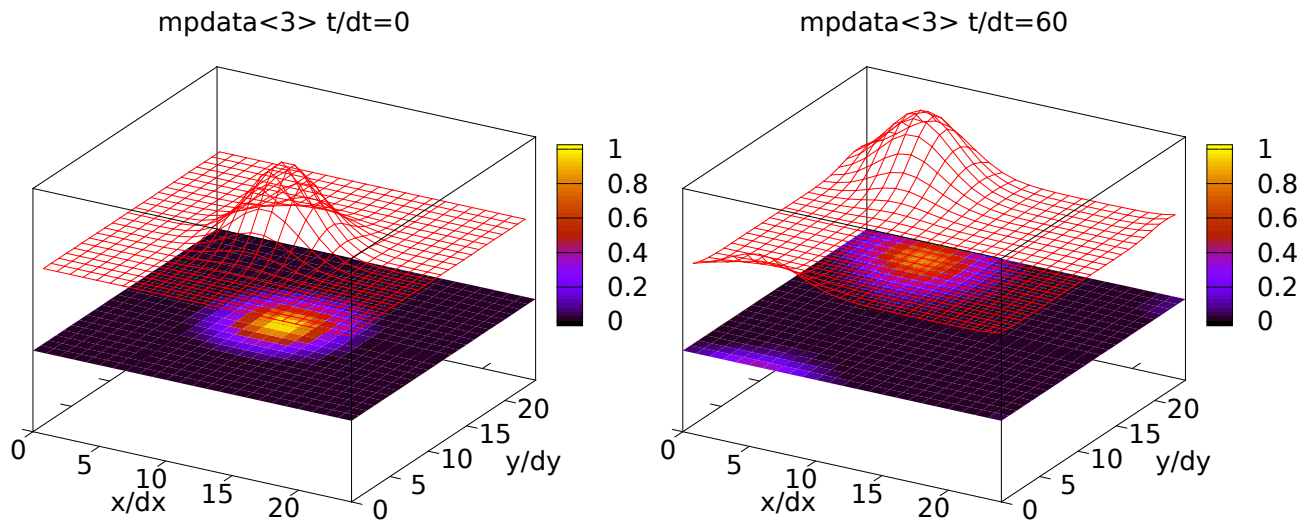

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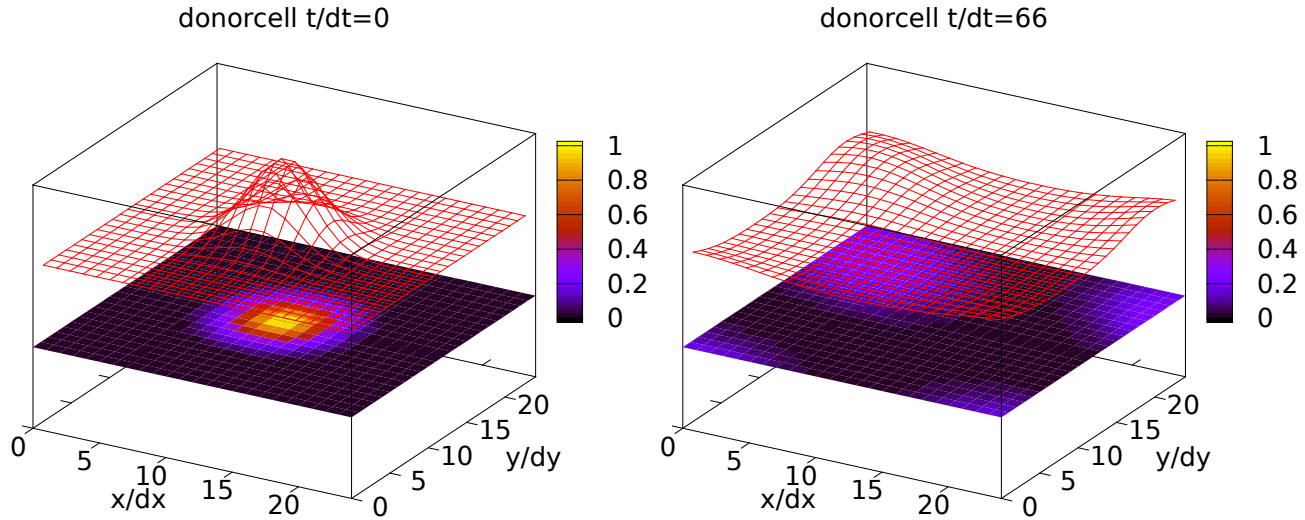

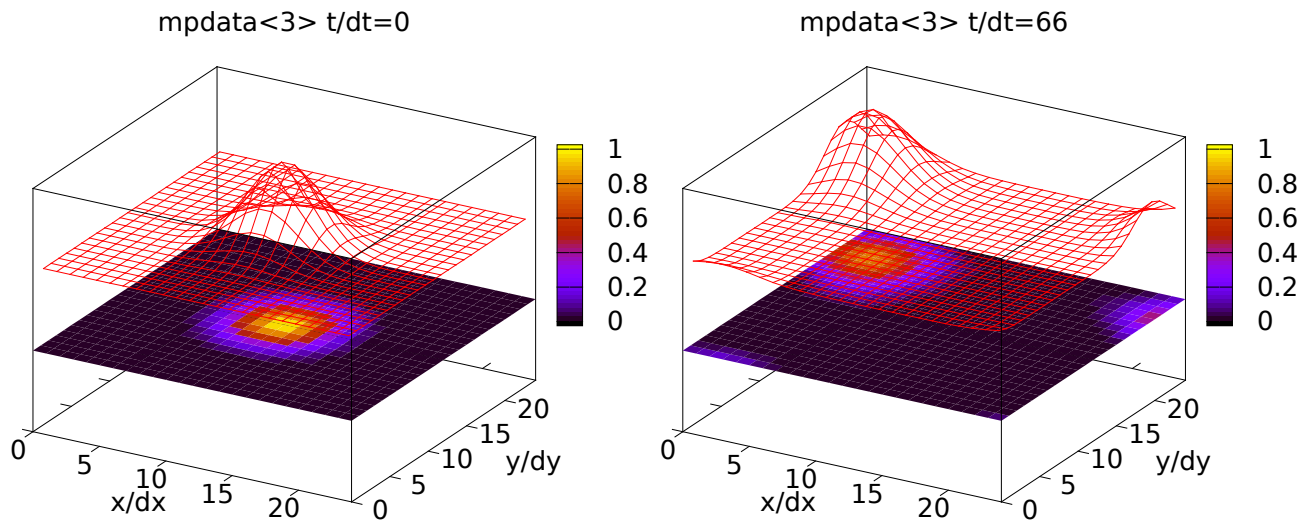

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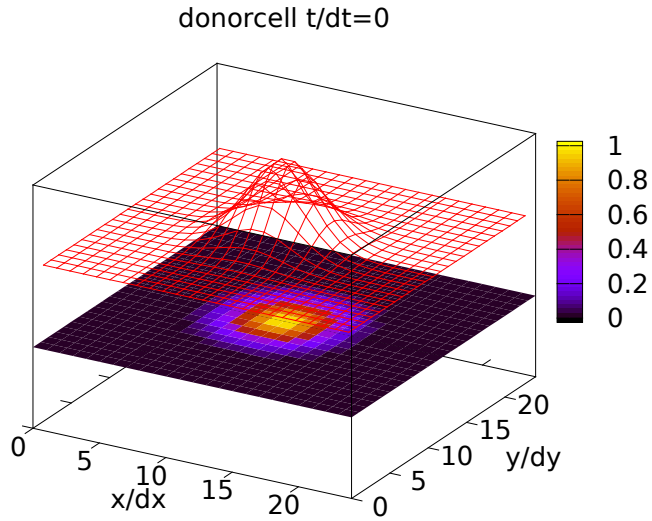

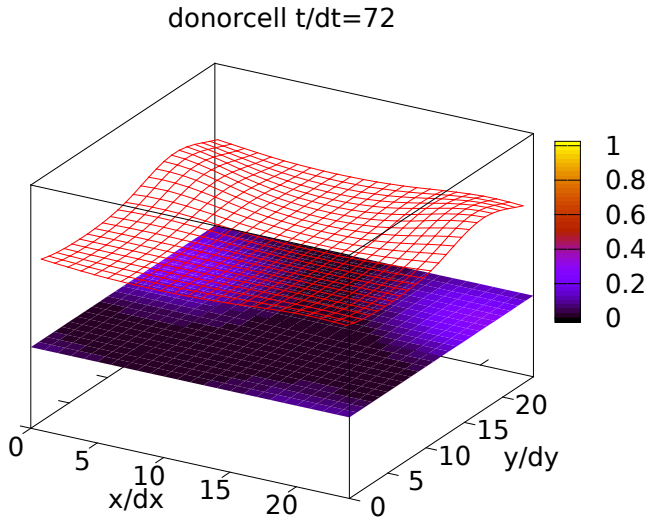

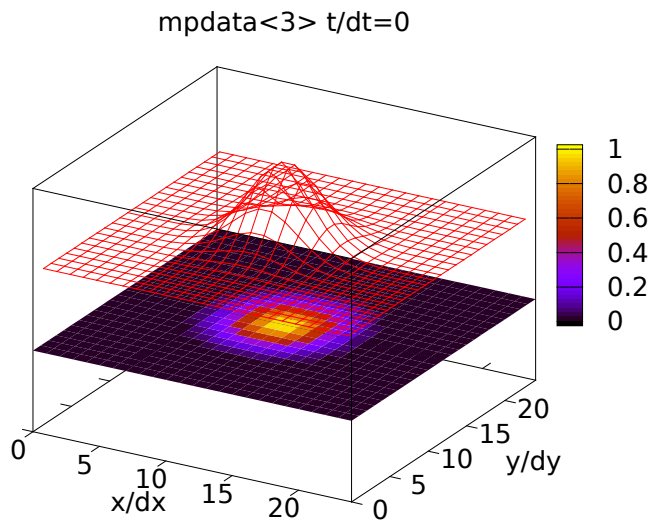

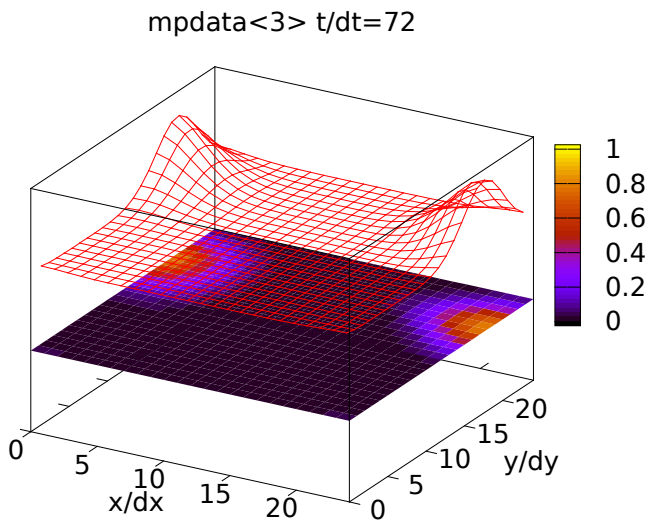

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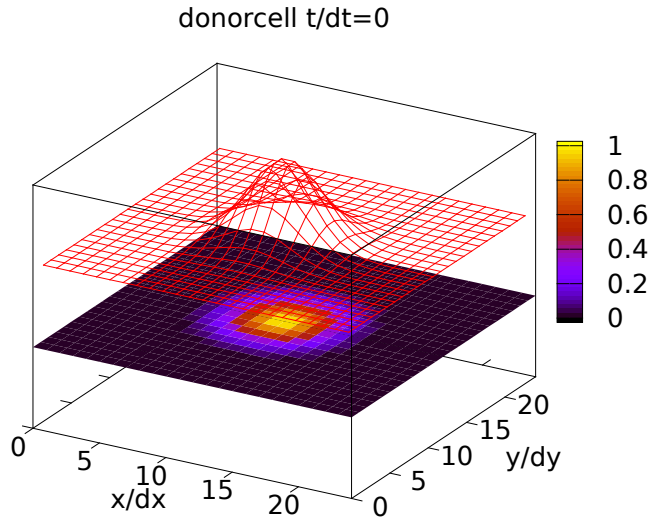

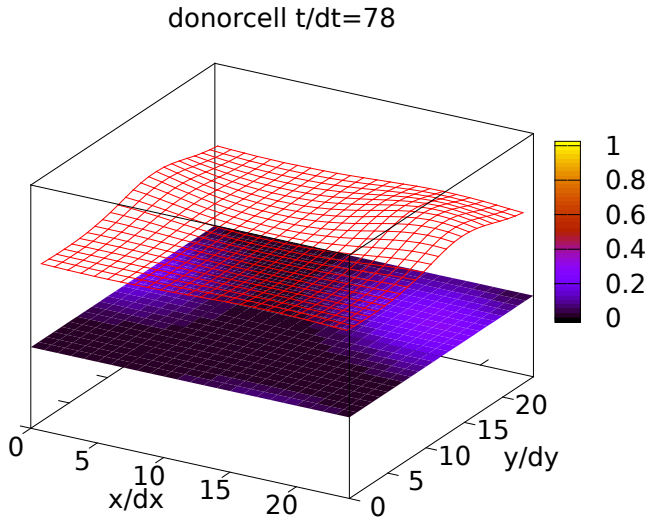

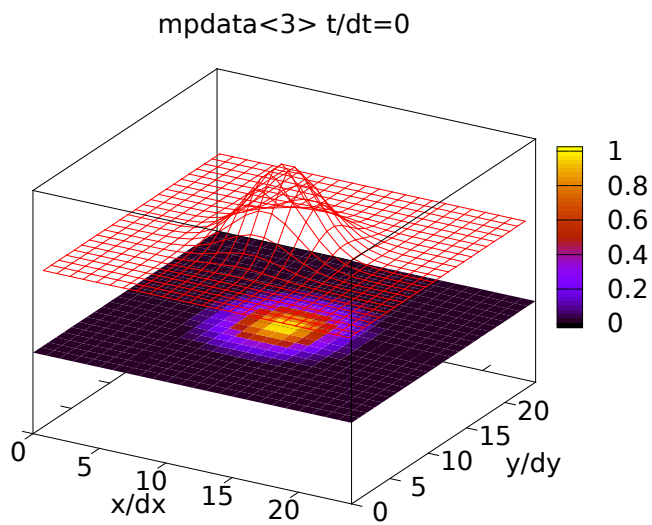

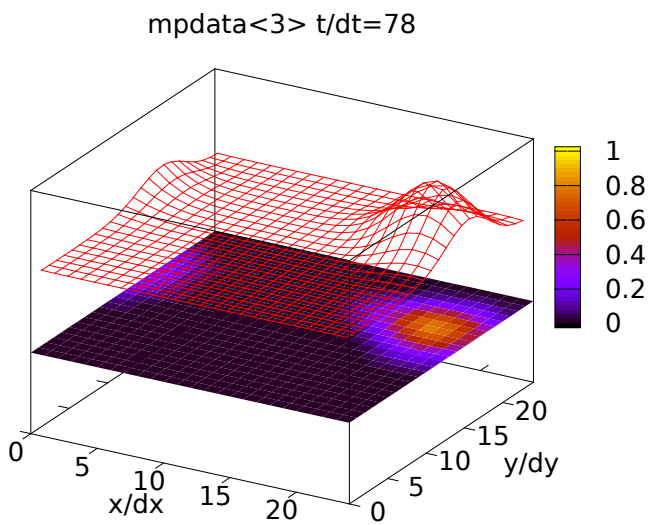

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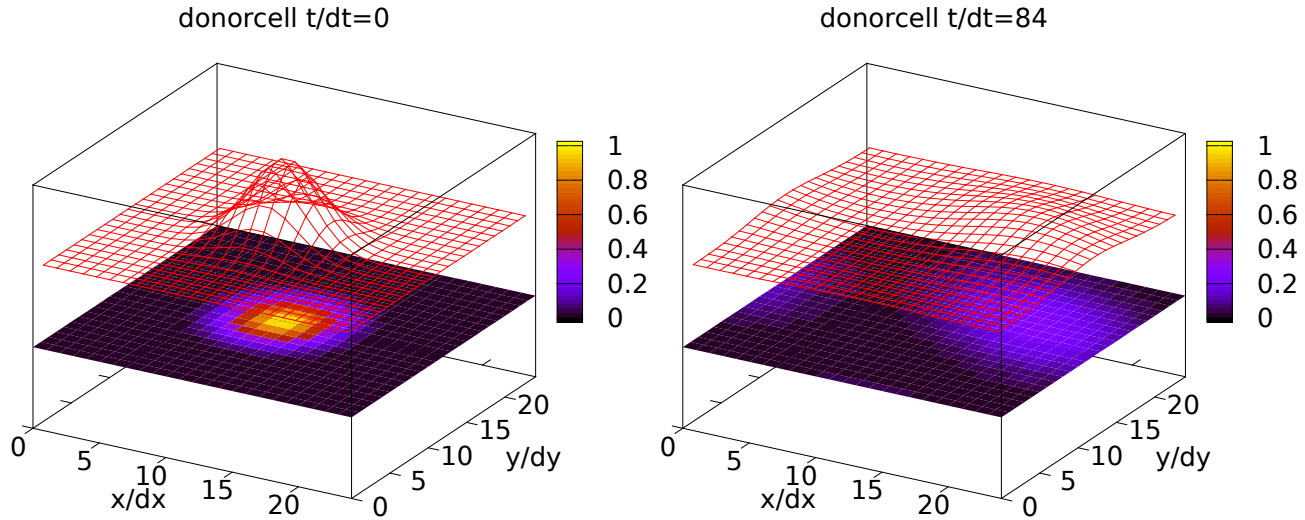

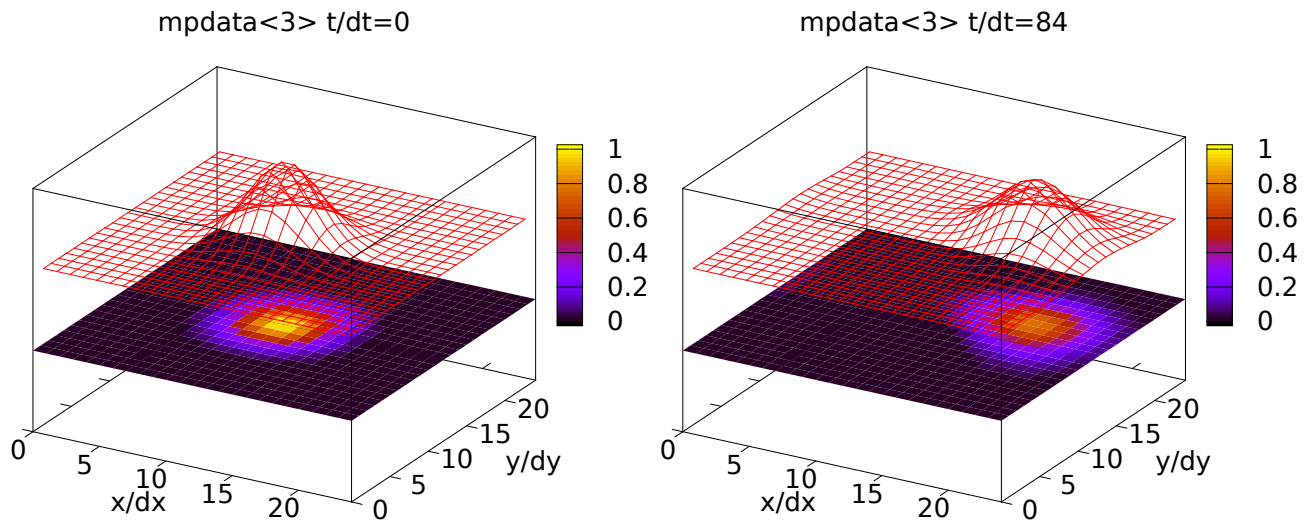

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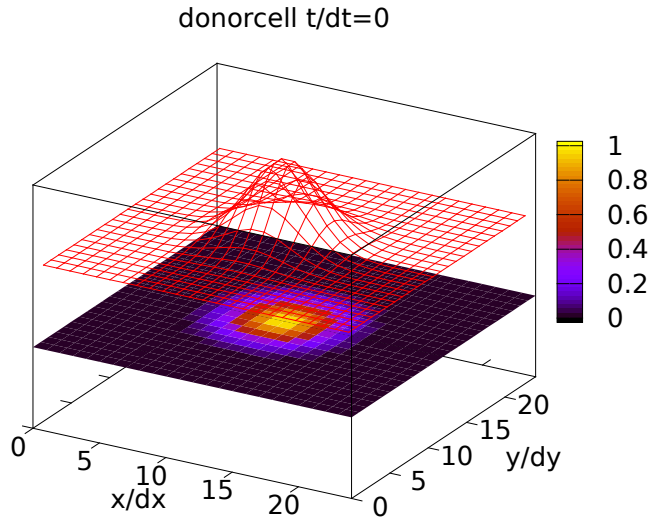

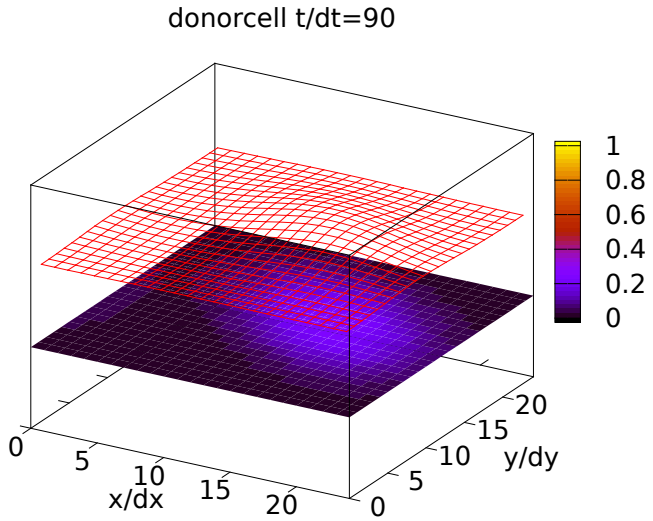

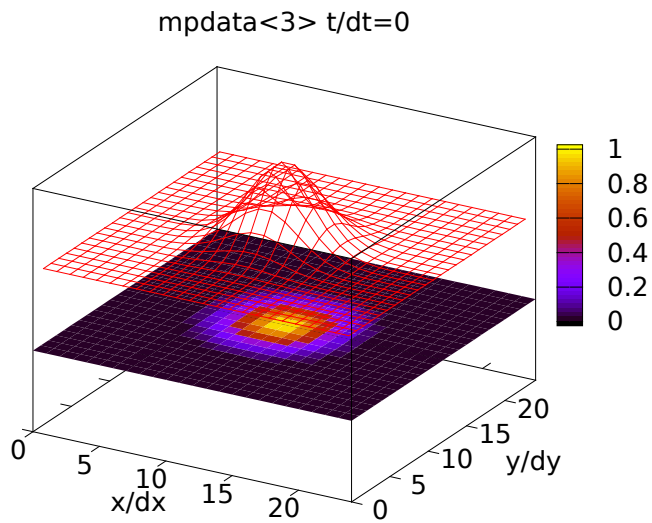

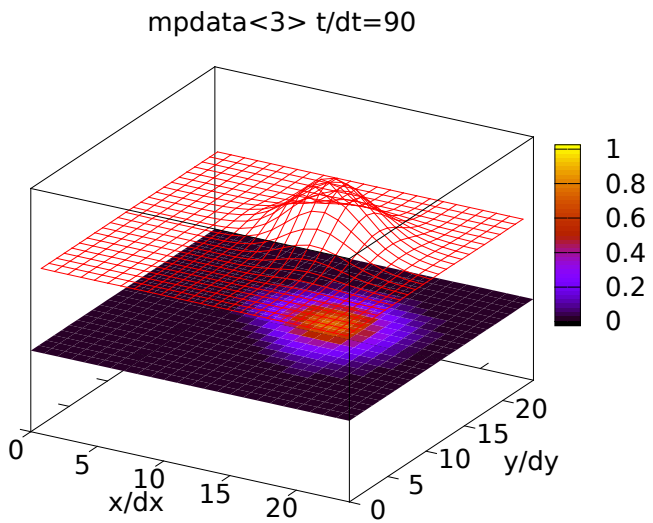

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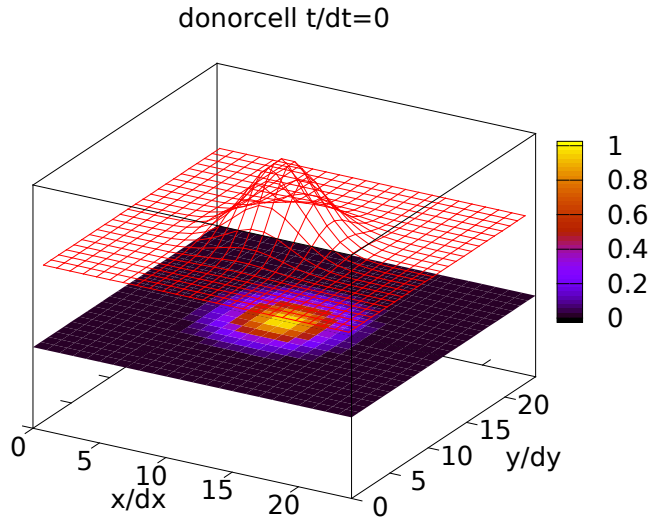

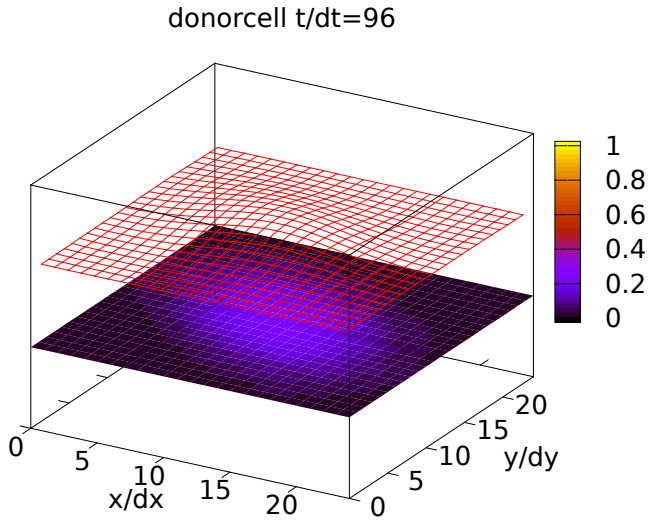

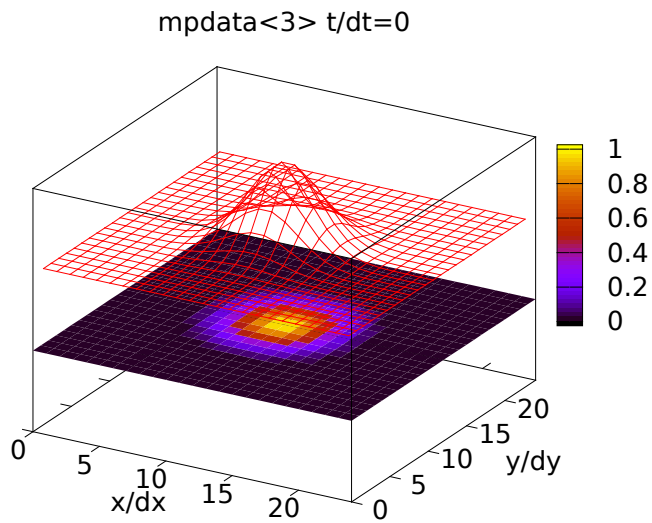

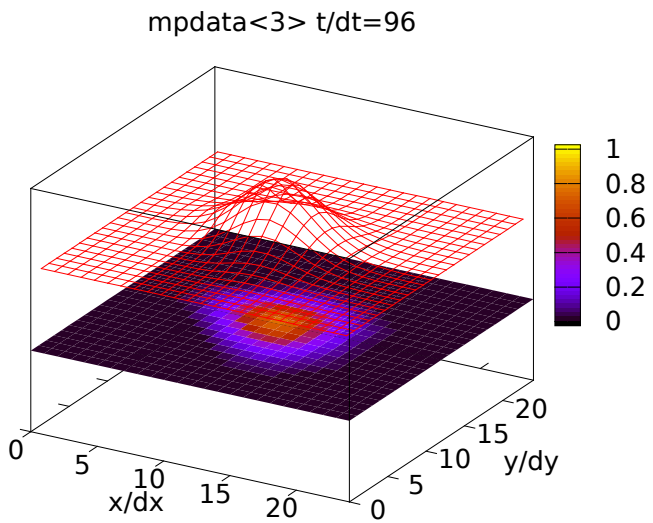

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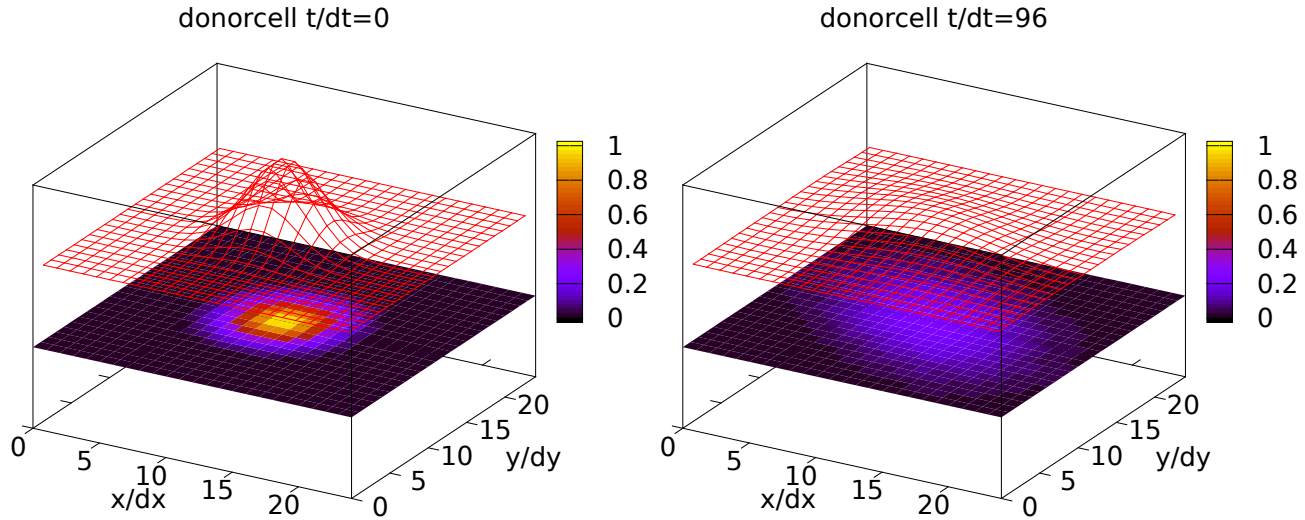

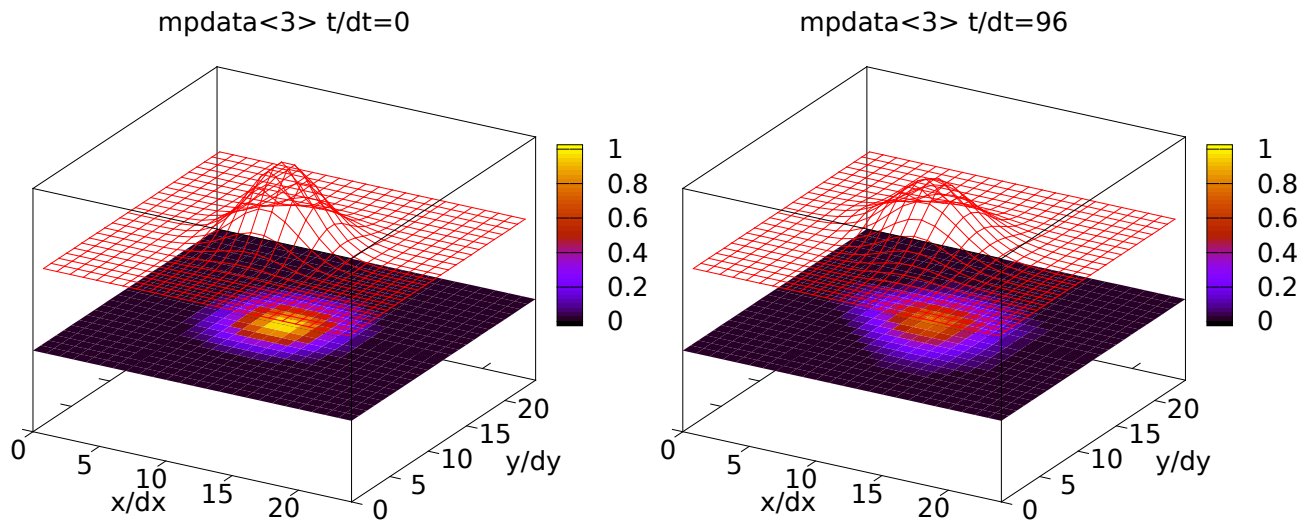

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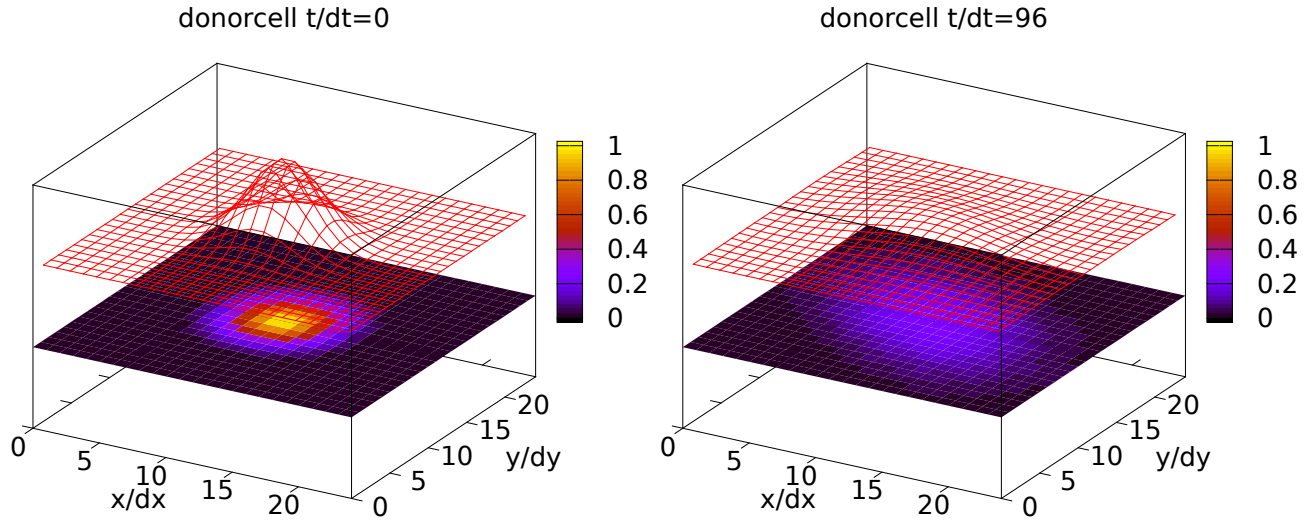

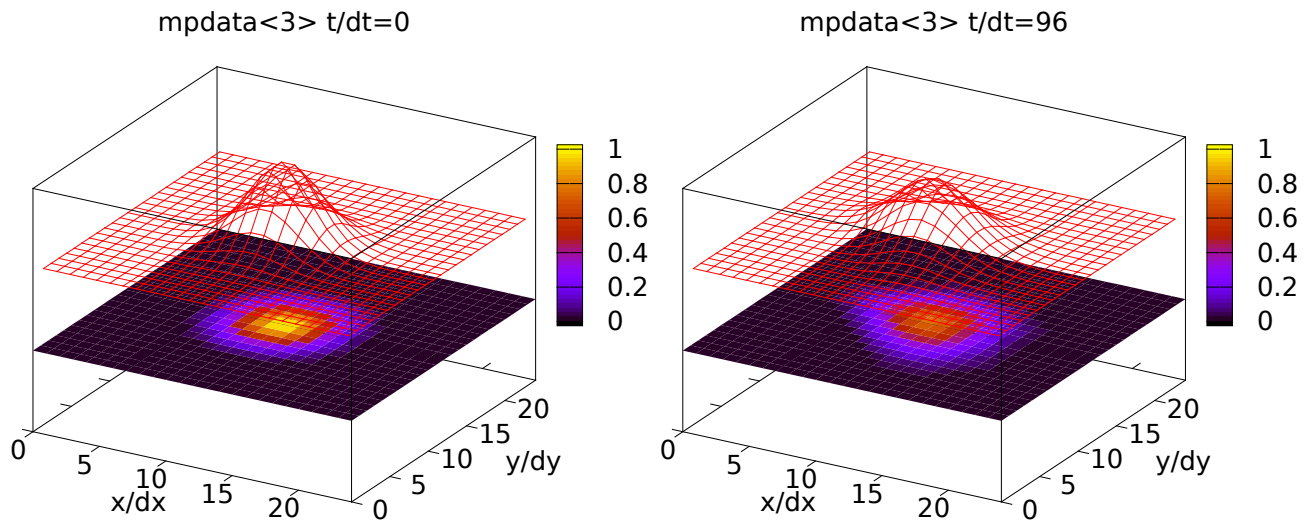

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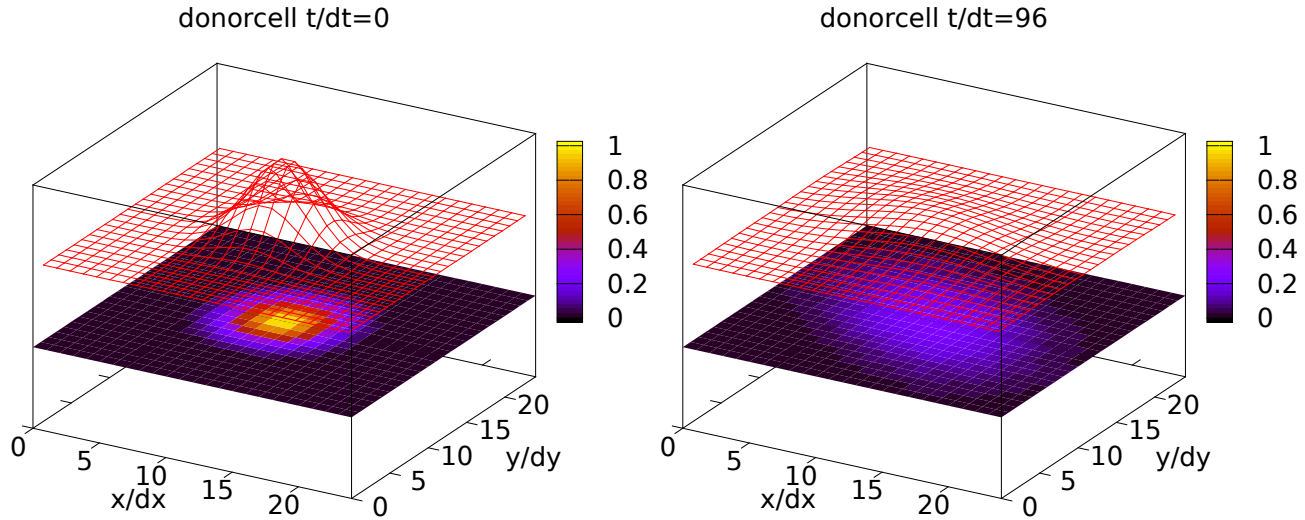

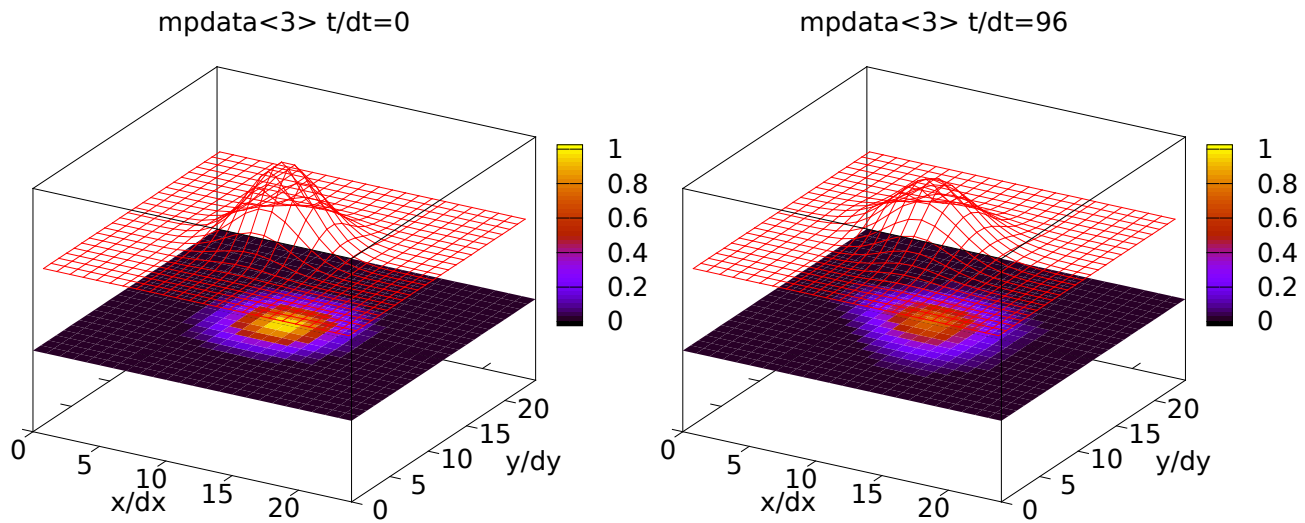

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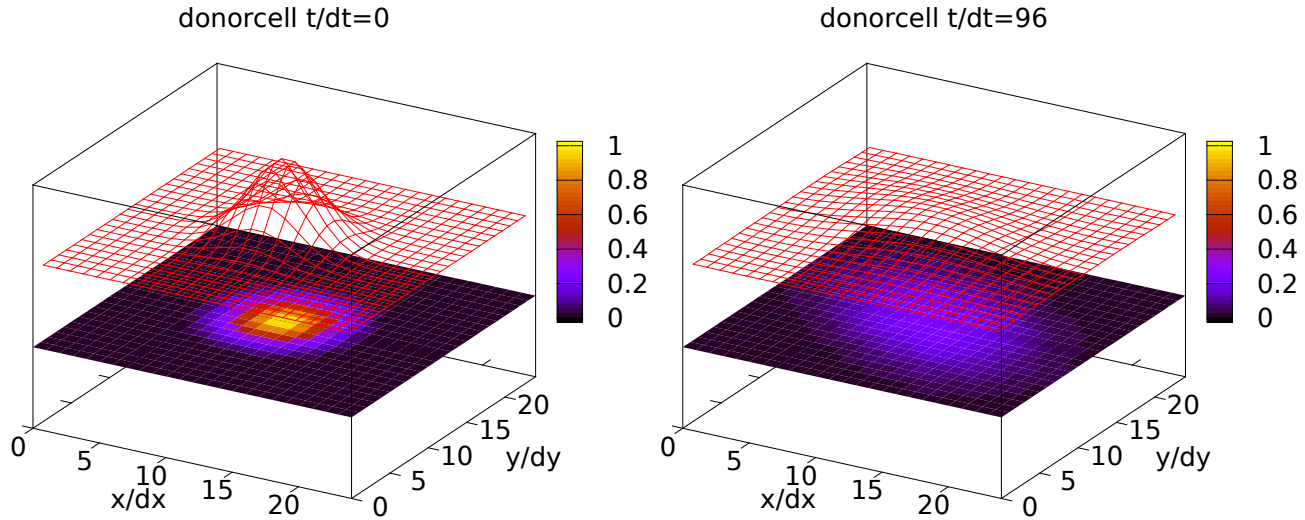

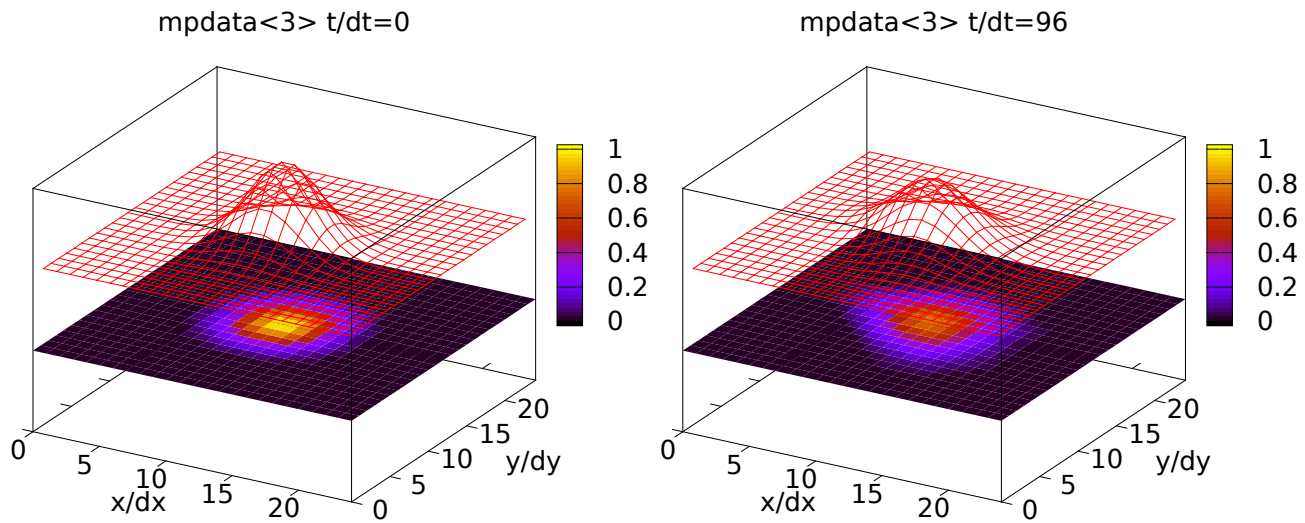

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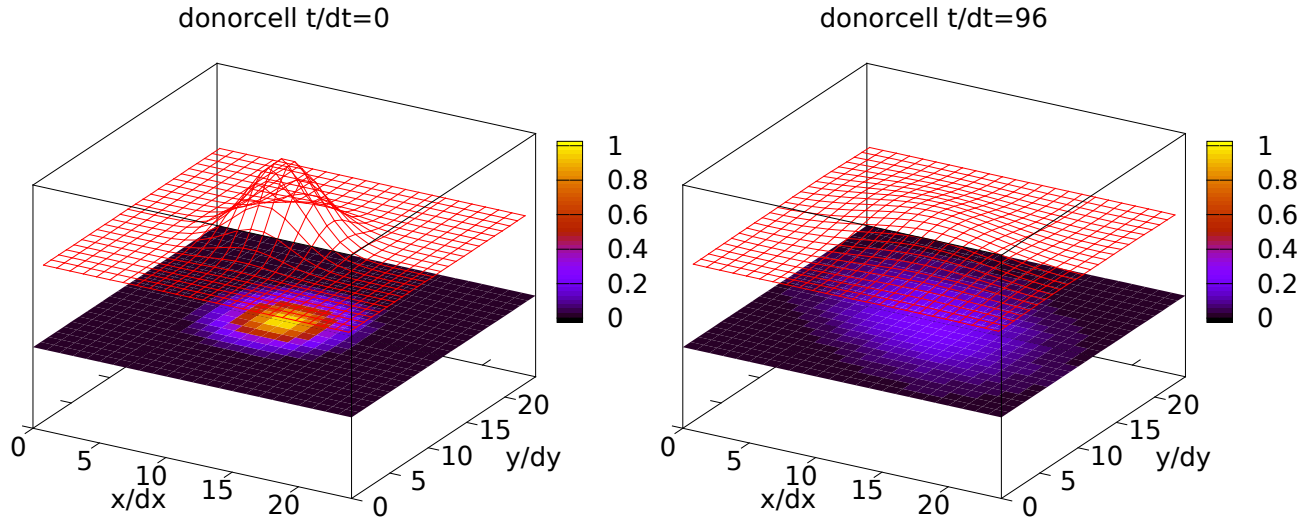

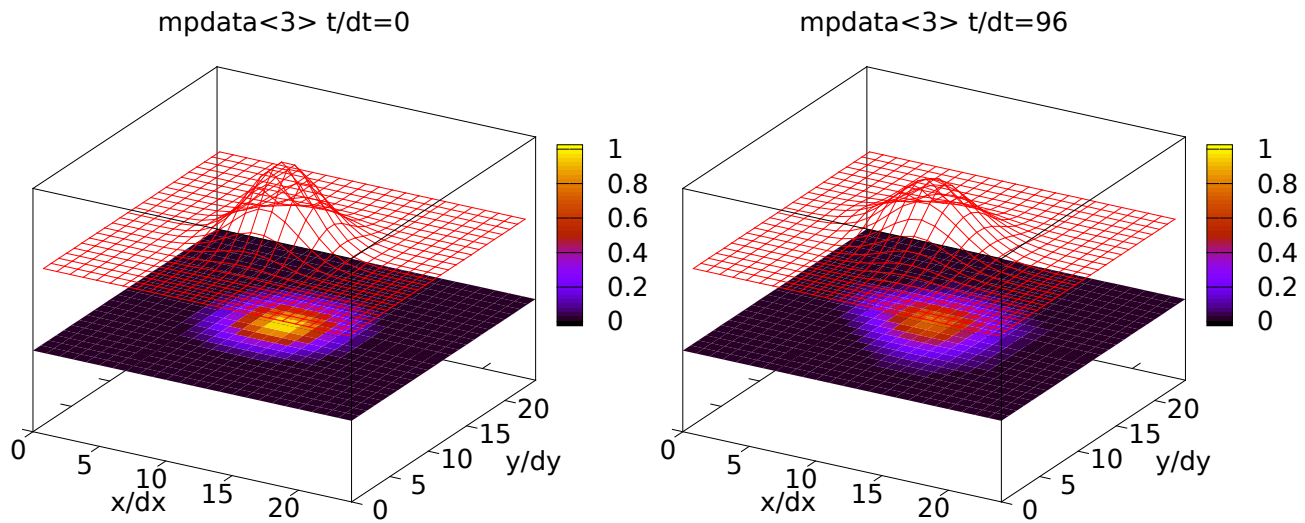

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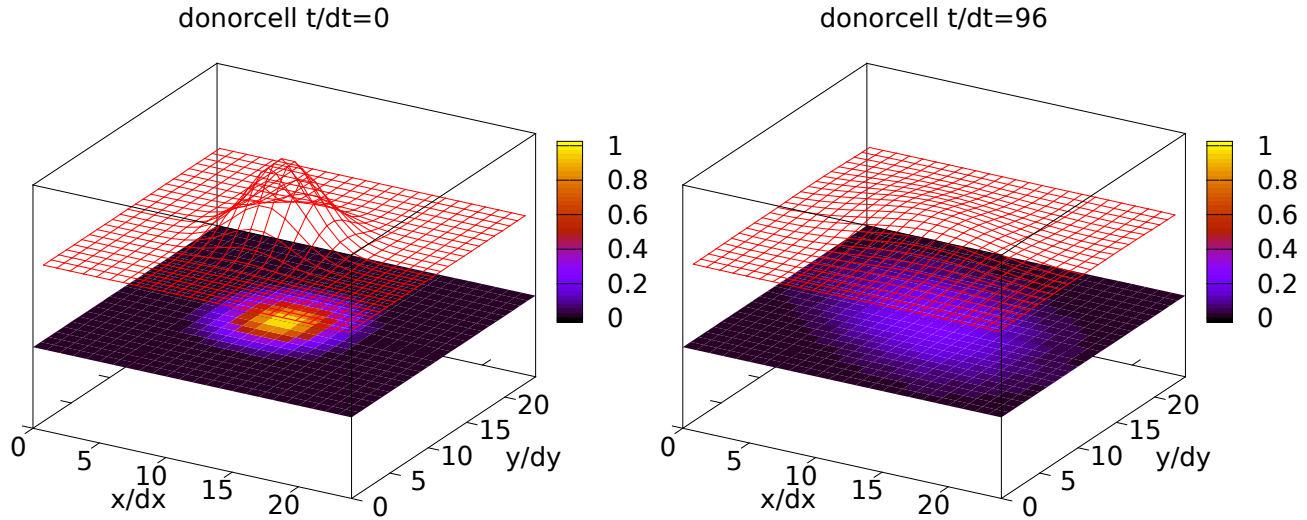

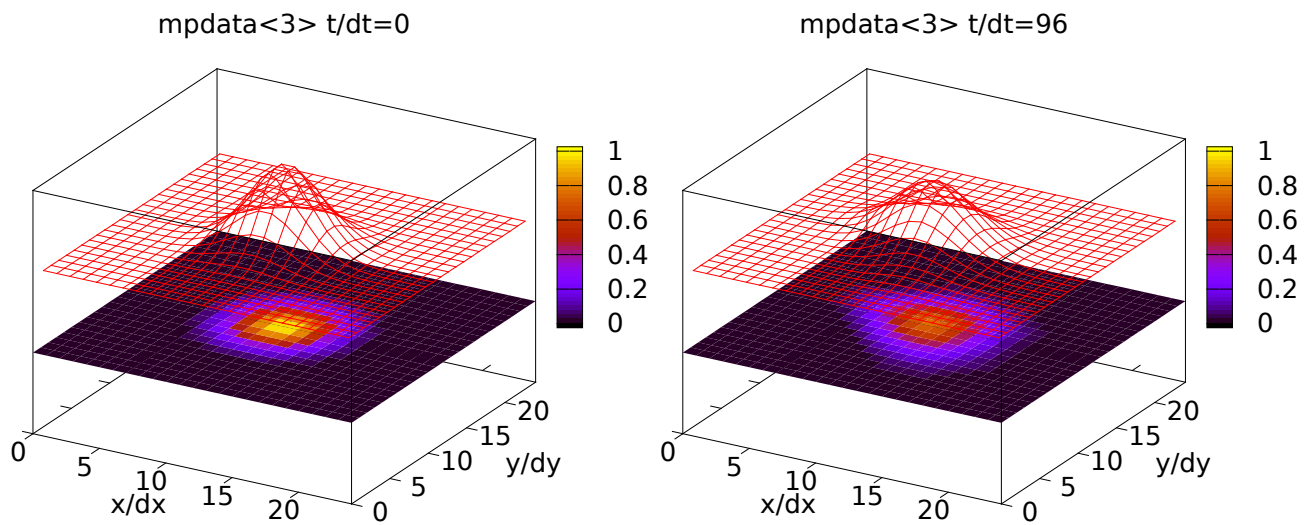

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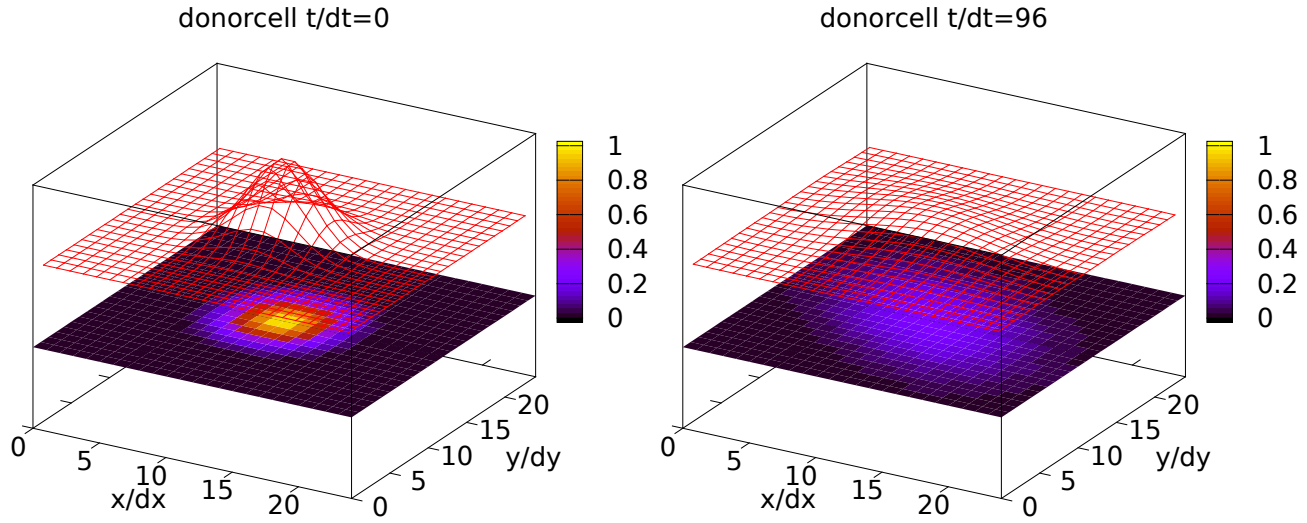

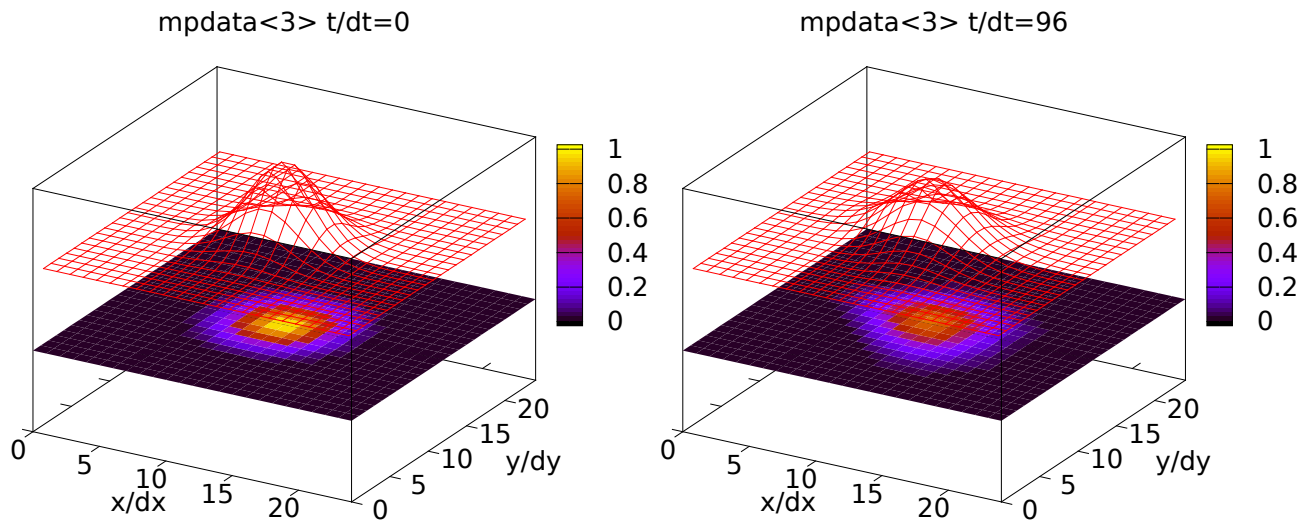

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MPDATA (Smolarkiewicz 1984) in formulæ

- advection equation: $\partial_t \psi = -\nabla \cdot (\vec{v}\psi)$
- two time-level forward-in-time scheme:

$$\psi^{[n+1]} = \psi^{[n]} - \sum_{\mathrm{d}} Adv(\psi^{[n]}, \vec{C})$$

$$\vec{C} = \vec{v} \cdot \frac{\Delta t}{\Delta x}$$

- donor-cell formula on an Arakawa-C grid:

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

$$F(\psi_L, \psi_R, C) = \max(C, 0) \cdot \psi_L + \min(C, 0) \cdot \psi_R = \frac{C + |C|}{2} \cdot \psi_L + \frac{C - |C|}{2} \cdot \psi_R$$

symbols:

ψ - conservative dependent variable (scalar field)

$\vec{C}$ - Courant number (vector field)

n - time level

d - dimension

i, j - grid indices

$\pi^d_{a,b}$ - permutation of (a,b) of order d

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MPDATA (Smolarkiewicz 1984) in formulæ

- MPDATA: corrective donor-cell steps using C':

$$C'^{[d]}_{[i,j]+\pi^d_{1/2,0}} = \left| C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \right| \cdot \left[1 - \left| C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \right| \right] \cdot A^{[d]}_{[i,j]}(\psi) - \sum_{q=0, q\neq d}^{N} C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \cdot \overline{C}^{[q]}_{[i,j]+\pi^d_{1/2,0}} \cdot B^{[d]}_{[i,j]}(\psi)$$

$$\overline{C}^{[q]}_{[i,j]+\pi^d_{1/2,0}} = \frac{1}{4} \cdot \left(C^{[q]}_{[i,j]+\pi^d_{1,1/2}} + C^{[q]}_{[i,j]+\pi^d_{0,1/2}} + C^{[q]}_{[i,j]+\pi^d_{1,-1/2}} + C^{[q]}_{[i,j]+\pi^d_{0,-1/2}} \right)$$

$$A^{[d]}_{[i,j]} = \frac{\psi_{[i,j]+\pi^d_{1,0}} - \psi_{[i,j]}}{\psi_{[i,j]+\pi^d_{1,0}} + \psi_{[i,j]}}$$

$$B^{[d]}_{[i,j]} = \frac{1}{2} \frac{\psi_{[i,j]+\pi^d_{1,1}} + \psi_{[i,j]+\pi^d_{0,1}} - \psi_{[i,j]+\pi^d_{1,-1}} - \psi_{[i,j]+\pi^d_{0,-1}}}{\psi_{[i,j]+\pi^d_{1,1}} + \psi_{[i,j]+\pi^d_{0,1}} + \psi_{[i,j]+\pi^d_{1,-1}} + \psi_{[i,j]+\pi^d_{0,-1}}}$$

- altogether: 0.06 kLOC in LaTeX

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MPDATA (Smolarkiewicz 1984) in formulæ

- MPDATA: corrective donor-cell steps using C':

$$C'^{[d]}_{[i,j]+\pi^d_{1/2,0}} = \left| C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \right| \cdot \left[1 - \left| C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \right| \right] \cdot A^{[d]}_{[i,j]}(\psi) - \sum_{q=0, q\neq d}^{N} C^{[d]}_{[i,j]+\pi^d_{1/2,0}} \cdot \overline{C}^{[q]}_{[i,j]+\pi^d_{1/2,0}} \cdot B^{[d]}_{[i,j]}(\psi)$$

$$\overline{C}^{[q]}_{[i,j]+\pi^d_{1/2,0}} = \frac{1}{4} \cdot \left(C^{[q]}_{[i,j]+\pi^d_{1,1/2}} + C^{[q]}_{[i,j]+\pi^d_{0,1/2}} + C^{[q]}_{[i,j]+\pi^d_{1,-1/2}} + C^{[q]}_{[i,j]+\pi^d_{0,-1/2}} \right)$$

$$A^{[d]}_{[i,j]} = \frac{\psi_{[i,j]+\pi^d_{1,0}} - \psi_{[i,j]}}{\psi_{[i,j]+\pi^d_{1,0}} + \psi_{[i,j]}}$$

$$B^{[d]}_{[i,j]} = \frac{1}{2} \frac{\psi_{[i,j]+\pi^d_{1,1}} + \psi_{[i,j]+\pi^d_{0,1}} - \psi_{[i,j]+\pi^d_{1,-1}} - \psi_{[i,j]+\pi^d_{0,-1}}}{\psi_{[i,j]+\pi^d_{1,1}} + \psi_{[i,j]+\pi^d_{0,1}} + \psi_{[i,j]+\pi^d_{1,-1}} + \psi_{[i,j]+\pi^d_{0,-1}}}$$

- **altogether: 0.06 kLOC in LaTeX**

symbols:

ψ - conservative dependent variable (scalar field)

$\vec{C}$ - Courant number (vector field)

n - time level

d - dimension

i, j - grid indices

$\pi^d_{a,b}$ - permutation of (a,b) of order d

MPDATA (Smolarkiewicz 1984) in formulæ

- "traditional" numerics:
  - floating-point arrays: ψ, $C^{[0]}$, $C^{[1]}$
  - integers: n, d, i, j
  - statements
  - ...
  - #LOC $\gg$ #LOC in LaTeX, human-readable?

- OO numerics:
  - instance of an array-of-floats class: ψ
  - instance of a vector-of-arrays class: C
  - instance of an array-index class: i, j
  - ...
  - instance of an array-valued-expression class: $\psi_{[i+1,j]} + \psi_{[i-1,j]}$
  - ...
  - how could it make one's life easier?
  - are there any solutions applicable in HPC?

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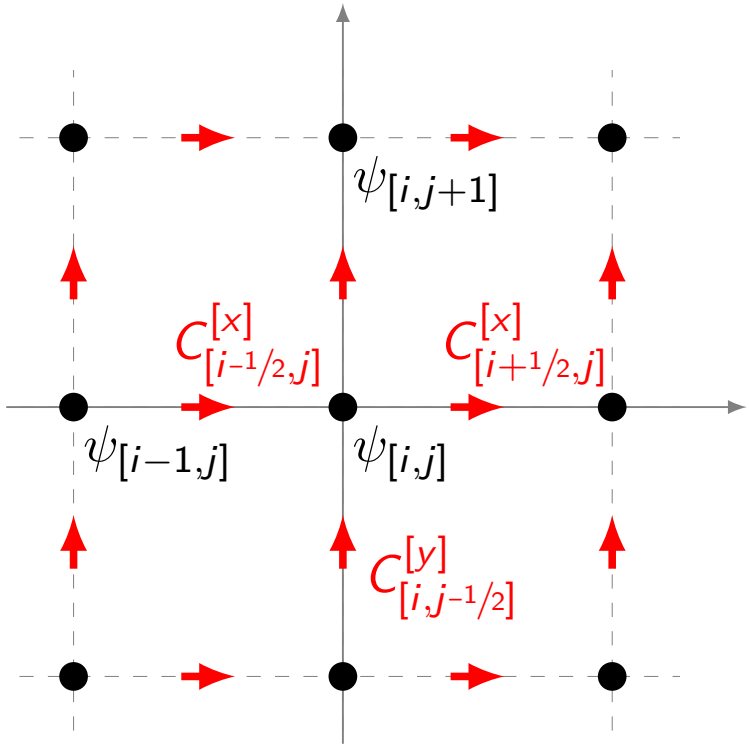
MPDATA in C++, Python and Fortran: prerequisites

OOP language/library set-ups for fast number crunching:
(in context of structured meshes, stencil-type algorithms)

- C++ & Blitz++
- Python & NumPy
- Fortran 200x
- ...[1]

[1] suggestions welcome on what else to try out

example (1/3): Arakawa-C grid fractional indices



example (1/3): Arakawa-C grid fractional indices

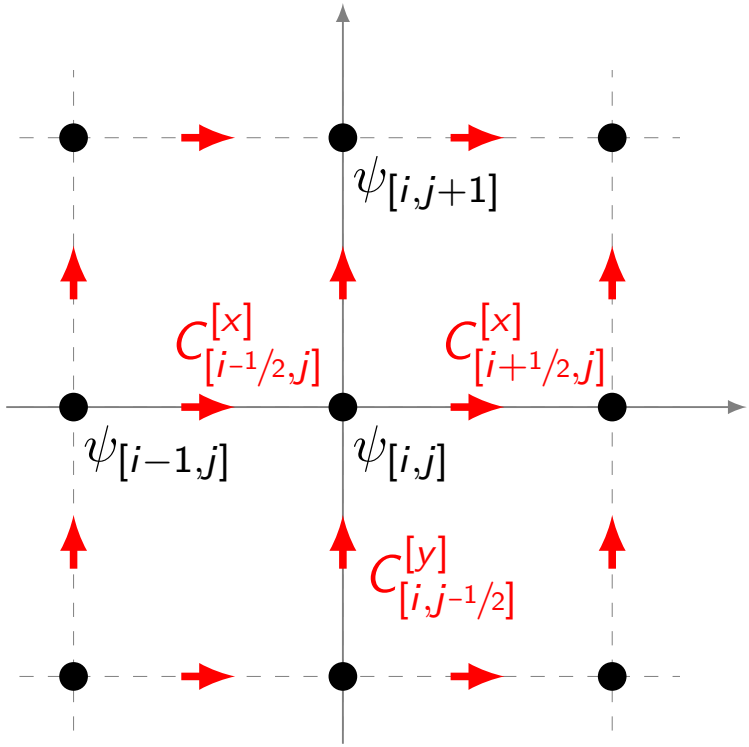
C++ / Blitz++:

(C++)

```
#include <blitz/array.h>
using arr_t = blitz::Array<real_t, 2>;
using rng_t = blitz::Range;
using idx_t = blitz::RectDomain<2>;
```

(C++)

```
struct hlf_t {} h;

inline rng_t operator+(const rng_t &i, const hlf_t &)
{
  return i;
}

inline rng_t operator-(const rng_t &i, const hlf_t &)
{
  return i-1;
}
```



example (1/3): Arakawa-C grid fractional indices

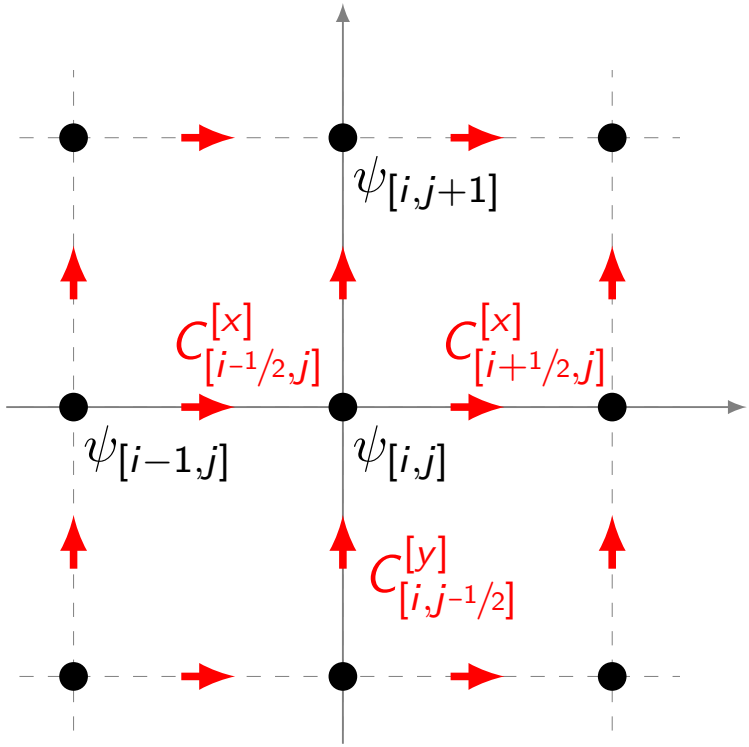
Python / NumPy:

(Python)

```
class shift():
  def __init__(self, plus, mnus):
    self.plus = plus
    self.mnus = mnus
  def __radd__(self, arg):
    return type(arg)(
      arg.start + self.plus,
      arg.stop  + self.plus
    )
  def __rsub__(self, arg):
    return type(arg)(
      arg.start - self.mnus,
      arg.stop  - self.mnus
    )
```

(Python)

```
one = shift(1,1)
hlf = shift(0,1)
```

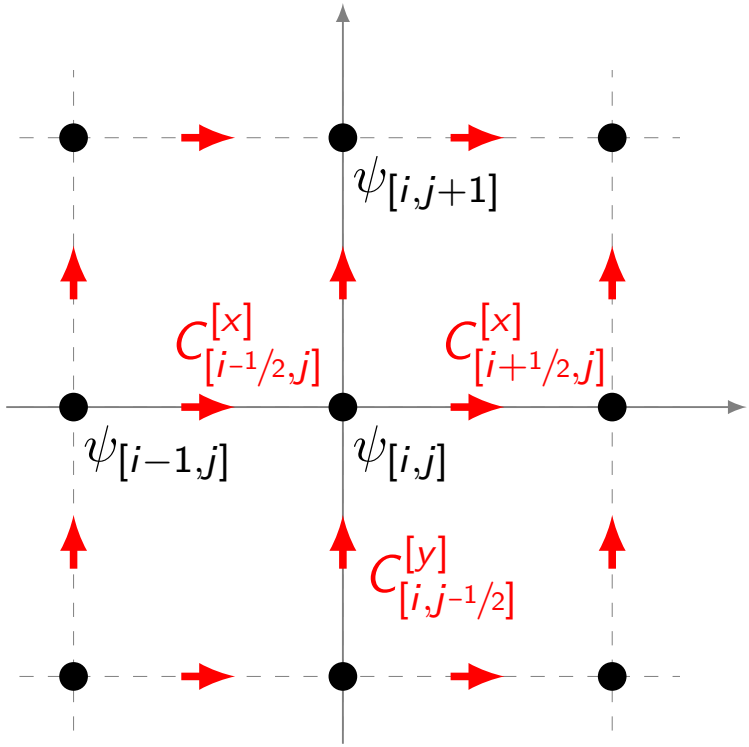


example (1/3): Arakawa-C grid fractional indices

Fortran:

(Fortran)

```
module arakawa_c_m
  implicit none

  type :: half_t
  end type

  type(half_t) :: h

  interface operator (+)
    module procedure ph
  end interface

  interface operator (-)
    module procedure mh
  end interface

  contains

  elemental function ph(i, h) result (return)
    integer, intent(in) :: i
    type(half_t), intent(in) :: h
    integer :: return
    return = i
  end function

  elemental function mh(i, h) result (return)
    integer, intent(in) :: i
    type(half_t), intent(in) :: h
    integer :: return
    return = i - 1
  end function
end module
```



example (2/3): dimensional indirection

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

C++ / Blitz++:

(C++)

```
template<int d>
inline auto donorcell(
  const arr_t &psi, const arr_t &C,
  const rng_t &i, const rng_t &j
) return_macro(
  F(
    psi(pi<d>(i,   j)),
    psi(pi<d>(i+1, j)),
      C(pi<d>(i+h, j))
  ) -
  F(
    psi(pi<d>(i-1, j)),
    psi(pi<d>(i,   j)),
      C(pi<d>(i-h, j))
  )
)
```

(C++)

```
void donorcell_op(
  const arrvec_t &psi, const int n,
  const arrvec_t &C,
  const rng_t &i, const rng_t &j
) {
  psi[n+1](i,j) = psi[n](i,j)
    - donorcell<0>(psi[n], C[0], i, j)
    - donorcell<1>(psi[n], C[1], j, i);
}
```

pi() returns an instance of blitz::RectDomain

example (2/3): dimensional indirection

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

Python / NumPy:

(Python)

```
def donorcell(d, psi, C, i, j):
  return (
    f(
      psi[pi(d, i,     j)],
      psi[pi(d, i+one, j)],
        C[pi(d, i+hlf, j)]
    ) -
    f(
      psi[pi(d, i-one, j)],
      psi[pi(d, i,     j)],
        C[pi(d, i-hlf, j)]
    )
  )
```

(Python)

```
def donorcell_op(psi, n, C, i, j):
  psi[n+1][i,j] = (psi[n][i,j]
    - donorcell(0, psi[n], C[0], i, j)
    - donorcell(1, psi[n], C[1], j, i)
  )
```

pi() returns a tuple of slices

example (2/3): dimensional indirection

Fortran:

(Fortran)

```
function donorcell(d, psi, C, i, j) result (return)
  integer :: d
  integer, intent(in) :: i(2), j(2)
  real(real_t) :: return(span(d, i, j), span(d, j, i))
  real(real_t), allocatable, intent(in) :: psi(:,:), C(:,:)
  return = (                                                &
    F(                                                      &
      pi(d, psi, i,   j),                                   &
      pi(d, psi, i+1, j),                                   &
      pi(d,   C, i+h, j)                                    &
    ) -                                                     &
    F(                                                      &
      pi(d, psi, i-1, j),                                   &
      pi(d, psi, i,   j),                                   &
      pi(d, C,   i-h, j)                                    &
    )                                                       &
  )
end function
```

(Fortran)

```
subroutine donorcell_op(psi, n, C, i, j)
  class(arrvec_t), allocatable :: psi
  class(arrvec_t), pointer :: C
  integer, intent(in) :: n
  integer, intent(in) :: i(2), j(2)

  real(real_t), pointer :: ptr(:,:)
  ptr => pi(0, psi%at(n+1)%p%a, i, j)
  ptr = pi(0, psi%at(n)%p%a, i, j)                          &
    - donorcell(0, psi%at(n)%p%a, C%at(0)%p%a, i, j)        &
    - donorcell(1, psi%at(n)%p%a, C%at(1)%p%a, j, i)
end subroutine
```

pi() returns pointer to a slab of an allocatable

example (3/3): array-valued functions

C++ / Blitz++:

(C++)

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

(C++)

```
template<class nom_t, class den_t>
inline auto mpdata_frac(
  const nom_t &nom, const den_t &den
) return_macro(
  where(den > 0, nom / den, 0)
)
```

(C++)

```
template<int d>
inline auto mpdata_A(const arr_t &psi,
  const rng_t &i, const rng_t &j
) return_macro(
  mpdata_frac(
    psi(pi<d>(i+1, j)) - psi(pi<d>(i,j)),
    psi(pi<d>(i+1, j)) + psi(pi<d>(i,j))
  )
)
```

$$A^{[d]}_{[i,j]} = \frac{\psi_{[i,j]+\pi^d_{1,0}} - \psi_{[i,j]}}{\psi_{[i,j]+\pi^d_{1,0}} + \psi_{[i,j]}}$$

return type: C++11's auto $\rightsquigarrow$ array expression

no temporary objects: by design

example (3/3): array-valued functions

Python / NumPy:

(Python)
```
def mpdata_frac(nom, den):
  return numpy.where(den > 0, nom/den, 0)
```

(Python)
```
def mpdata_A(d, psi, i, j):
  return mpdata_frac(
    psi[pi(d, i+one, j)] - psi[pi(d, i, j)],
    psi[pi(d, i+one, j)] + psi[pi(d, i, j)]
  )
```

$$A^{[d]}_{[i,j]} = \frac{\psi_{[i,j]+\pi^d_{1,0}} - \psi_{[i,j]}}{\psi_{[i,j]+\pi^d_{1,0}} + \psi_{[i,j]}}$$

return type: n/a

temporary objects: interpreter-dependant

example (3/3): array-valued functions

Fortran:

(Fortran)

```
function mpdata_frac(nom, den) result (return)
  real(real_t), intent(in) :: nom(:,:), den(:,:)
  real(real_t) :: return(size(nom, 1), size(nom, 2))
  where (den > 0)
    return = nom / den
  elsewhere
    return = 0
  end where
end function
```

(Fortran)

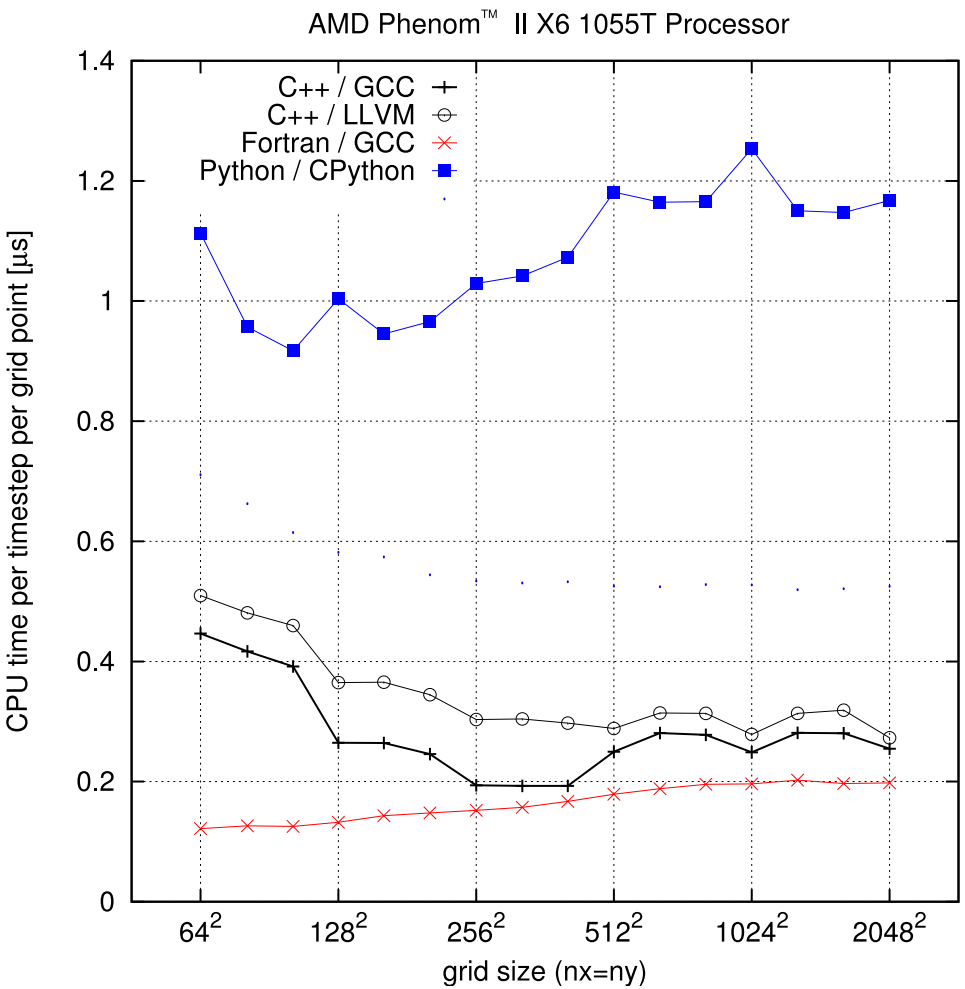
```
function mpdata_A(d, psi, i, j) result (return)
  integer :: d
  real(real_t), allocatable, intent(in) :: psi(:,:)
  integer, intent(in) :: i(2), j(2)
  real(real_t) :: return(span(d, i, j), span(d, j, i))
  return = mpdata_frac(                                  &
    pi(d, psi, i+1, j) - pi(d, psi, i, j),               &
    pi(d, psi, i+1, j) + pi(d, psi, i, j)                &
  )
end function
```

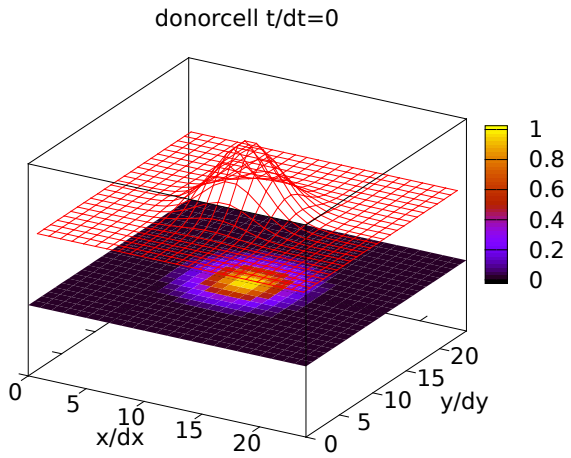
$$A^{[d]}_{[i,j]} = \frac{\psi_{[i,j]+\pi^d_{1,0}} - \psi_{[i,j]}}{\psi_{[i,j]+\pi^d_{1,0}} + \psi_{[i,j]}}$$

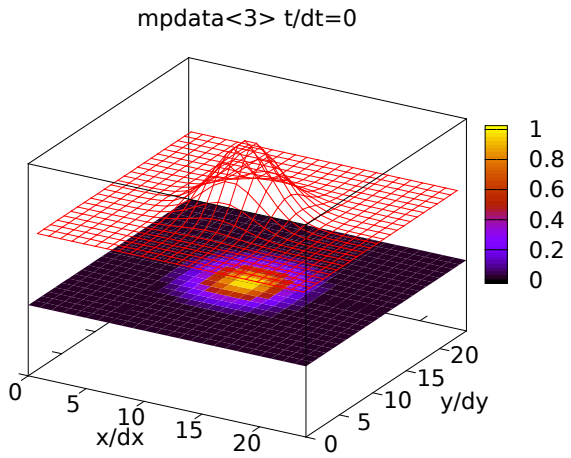
return type: "dimension" (array)

temporary objects: compiler-dependant

MPDATA in C++, Python and Fortran: performance







Is there any way to improve Python's performance?

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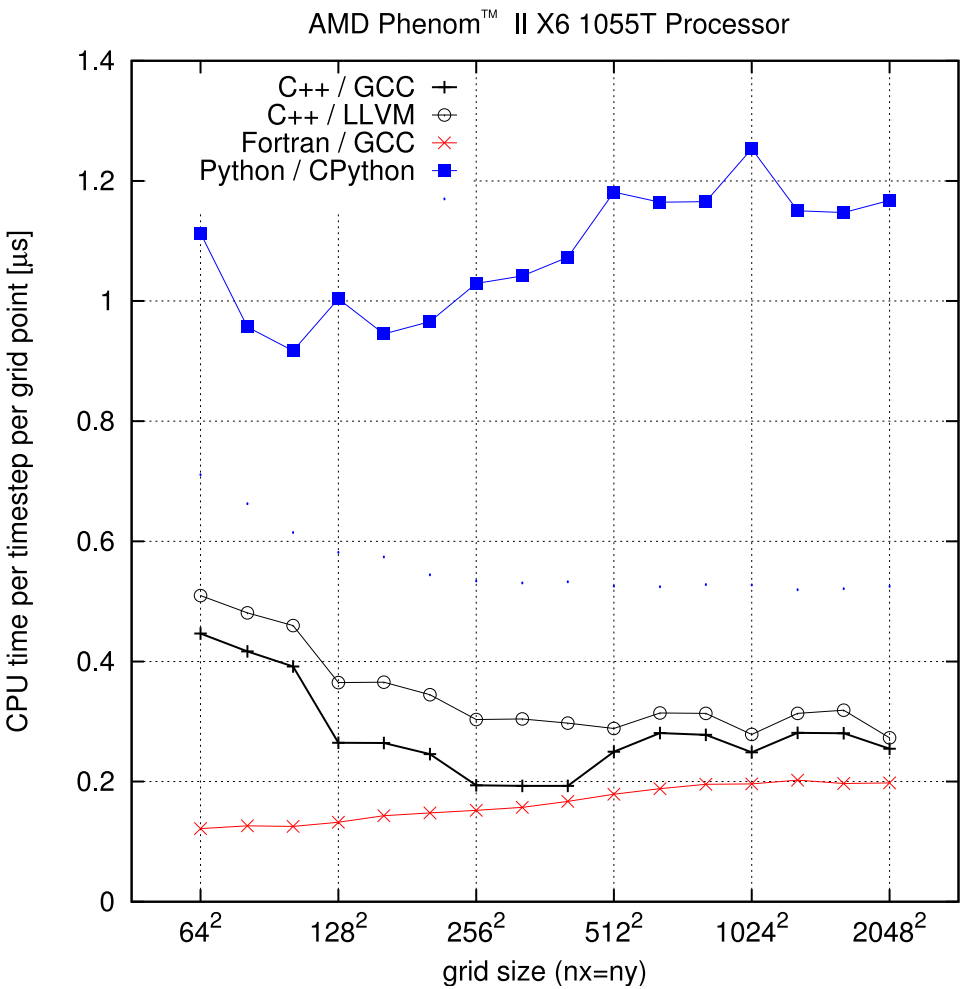

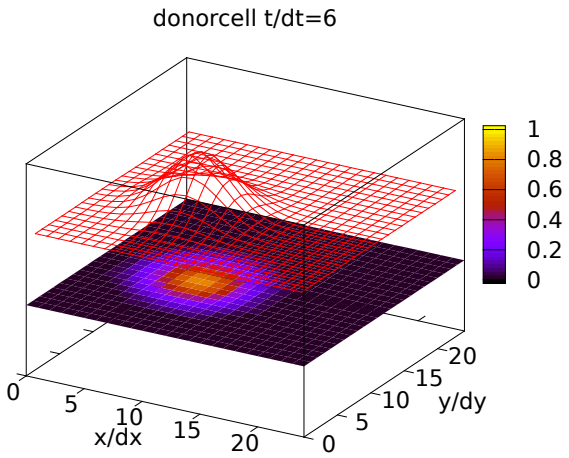

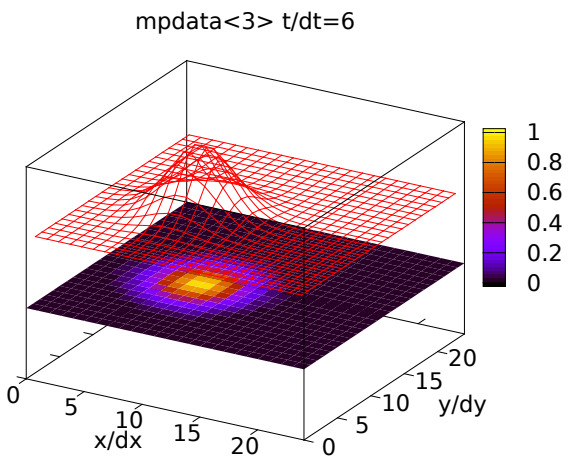

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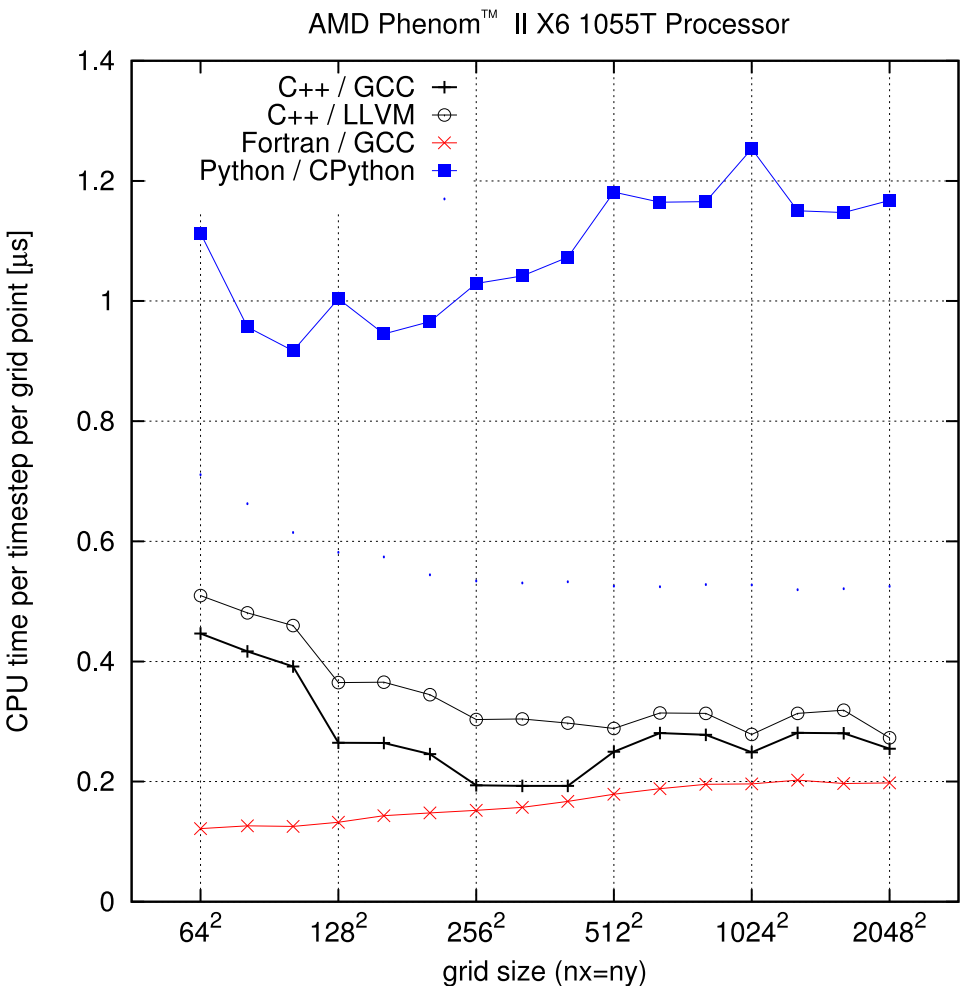

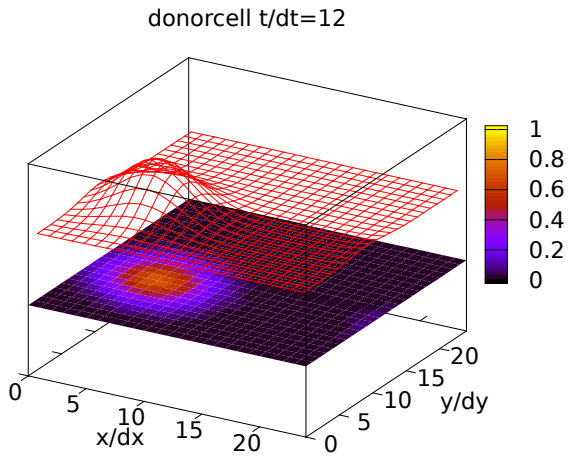

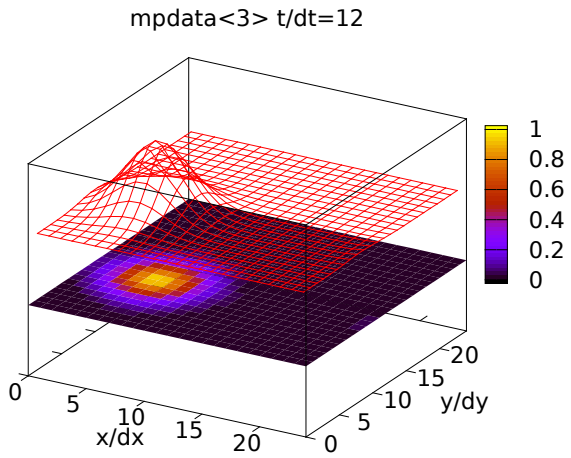

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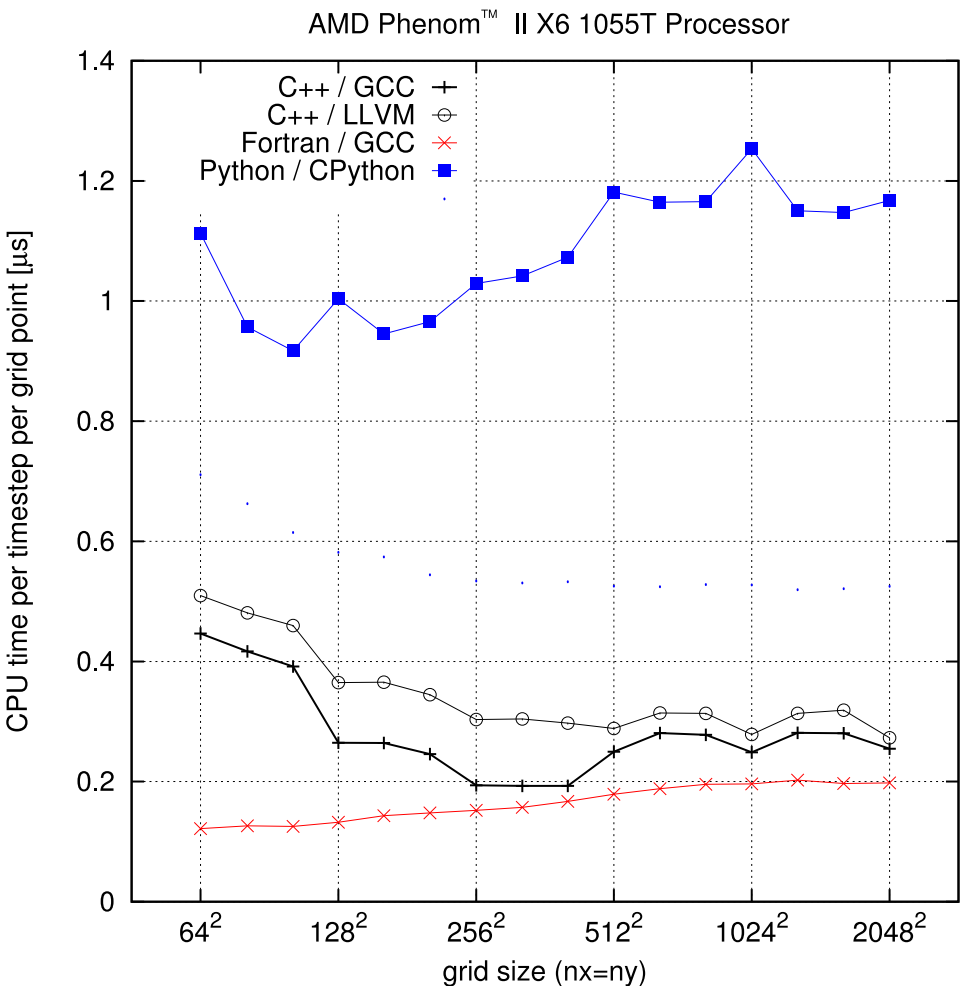

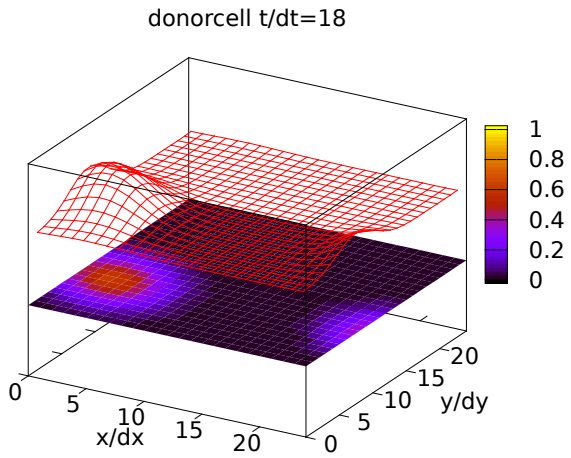

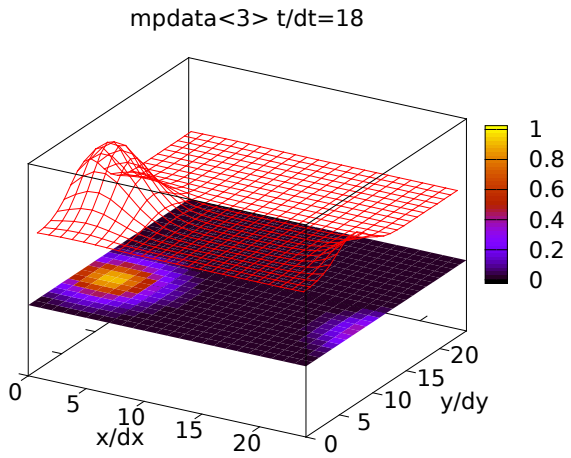

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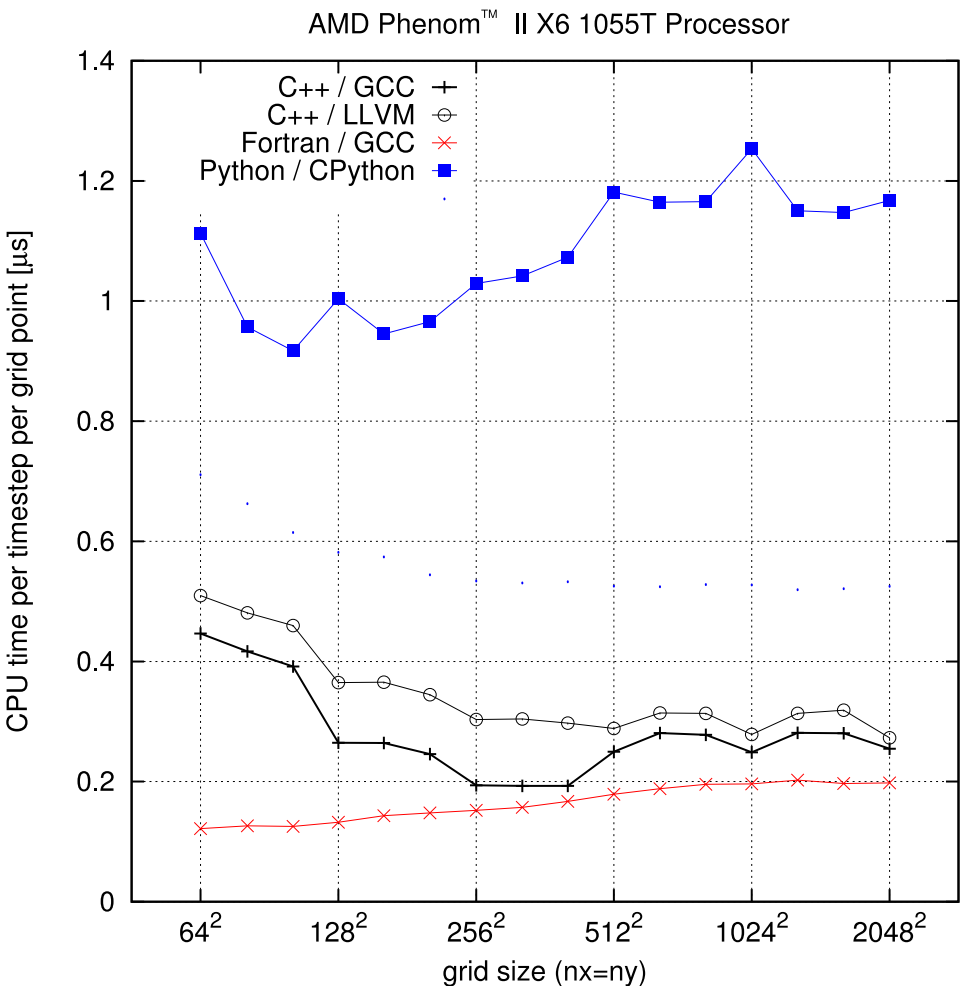

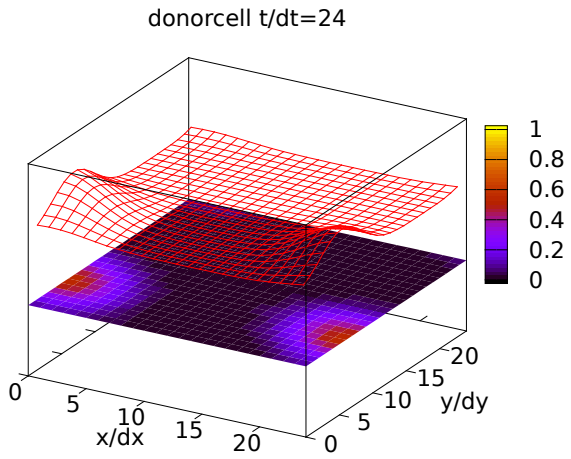

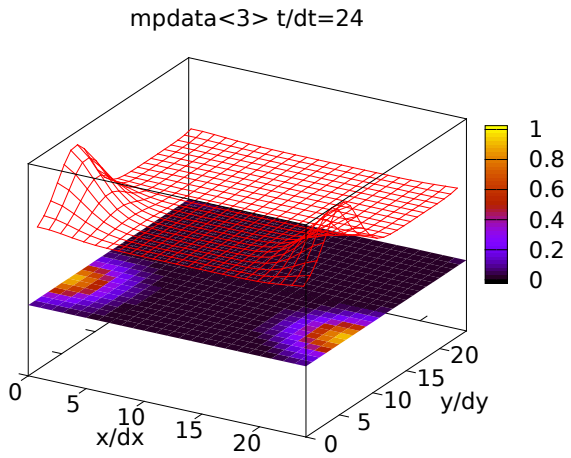

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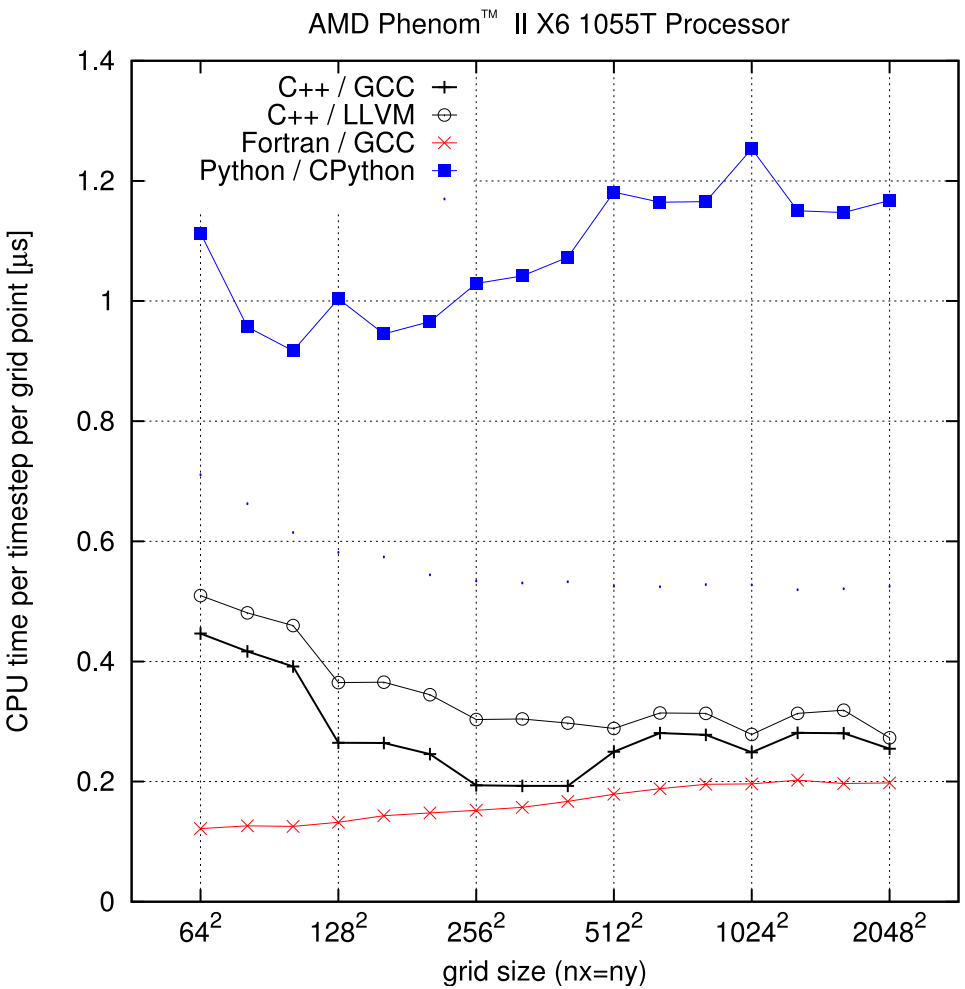

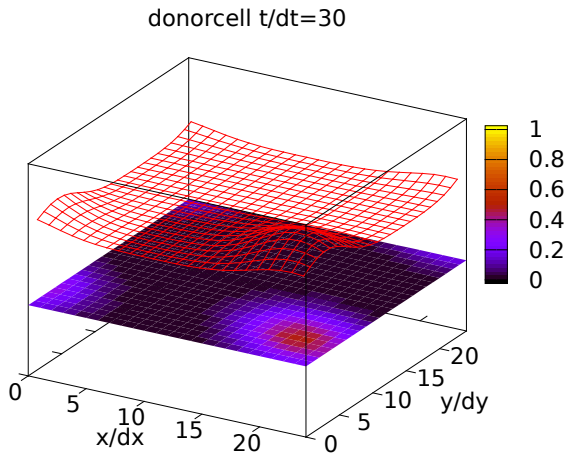

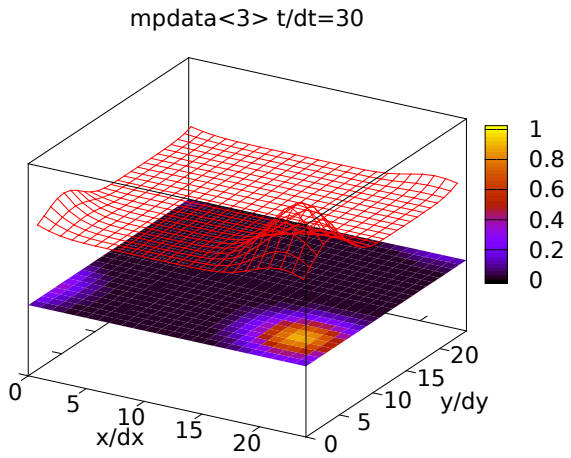

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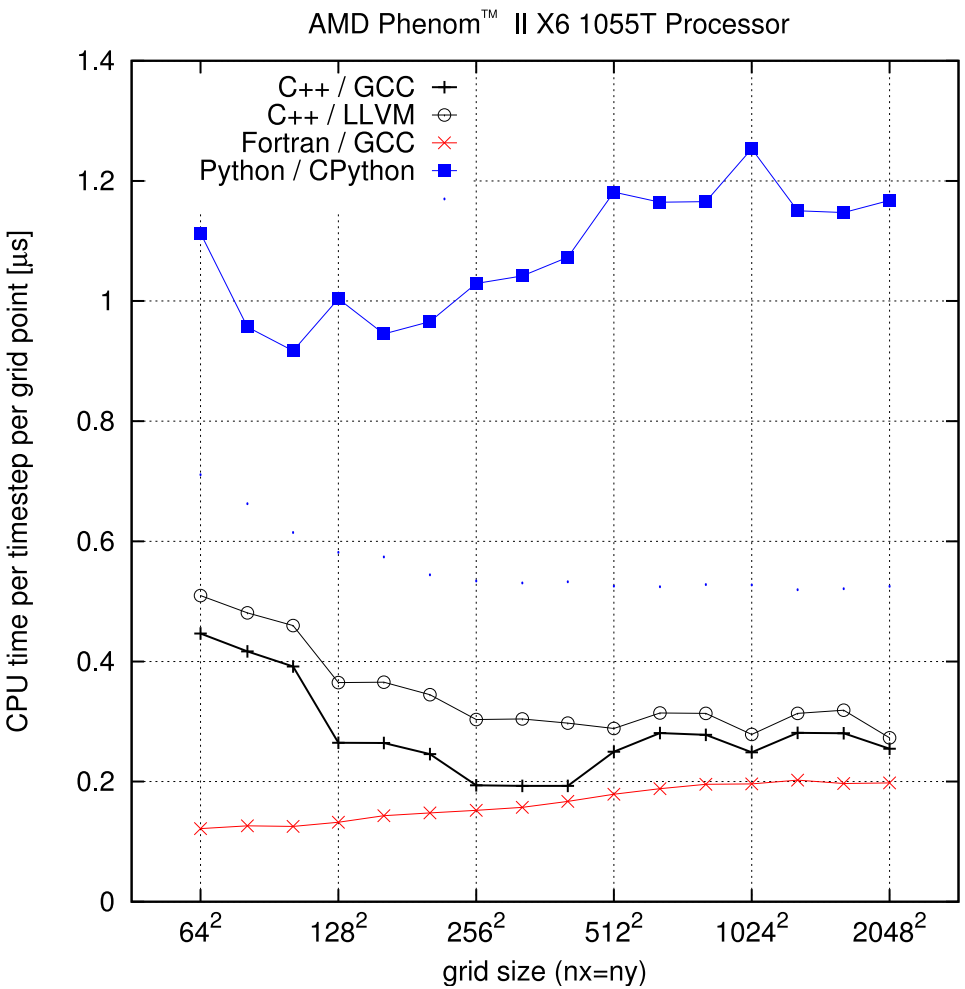

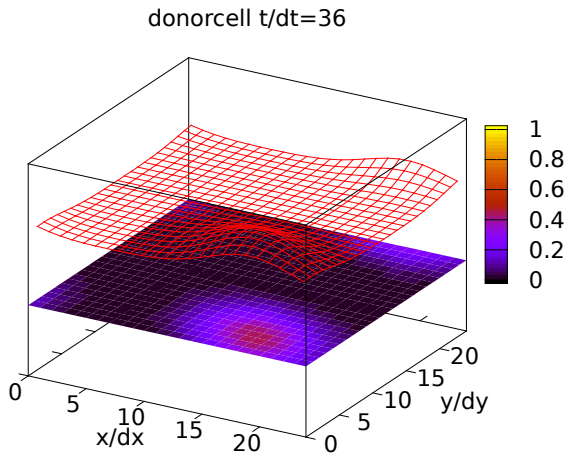

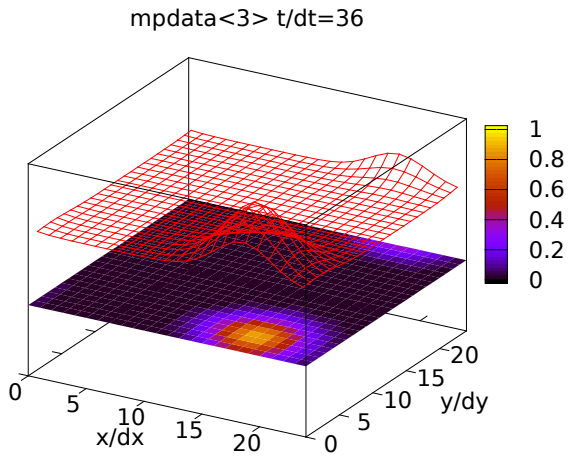

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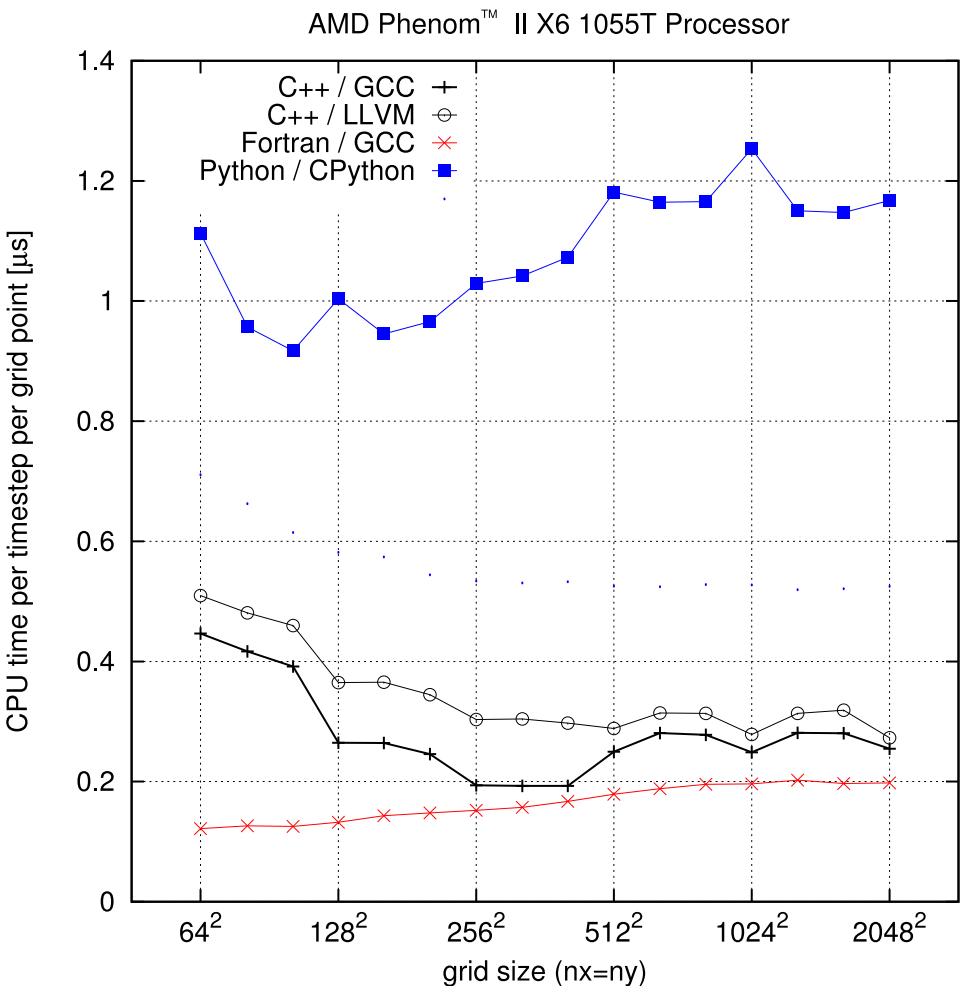

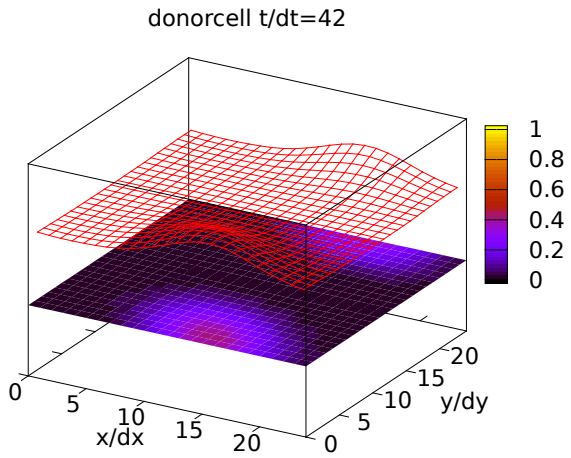

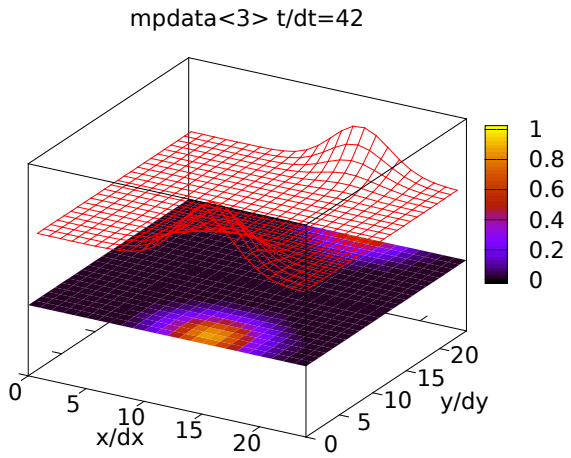

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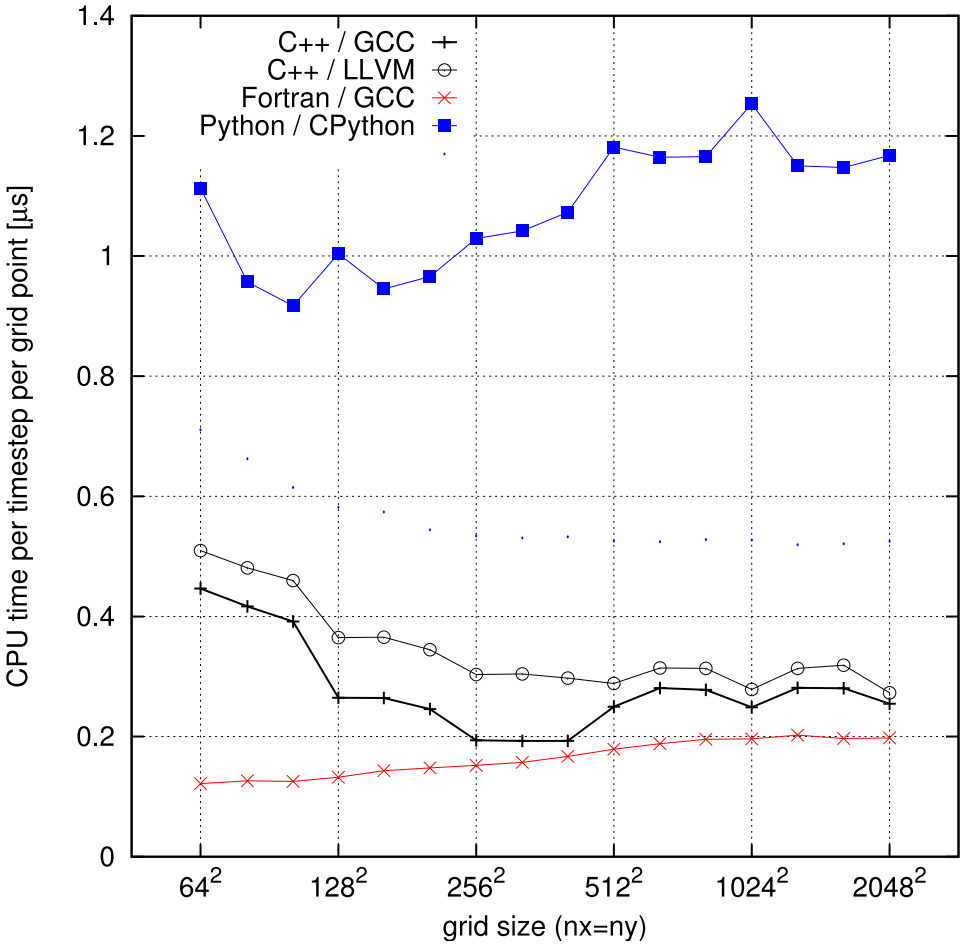

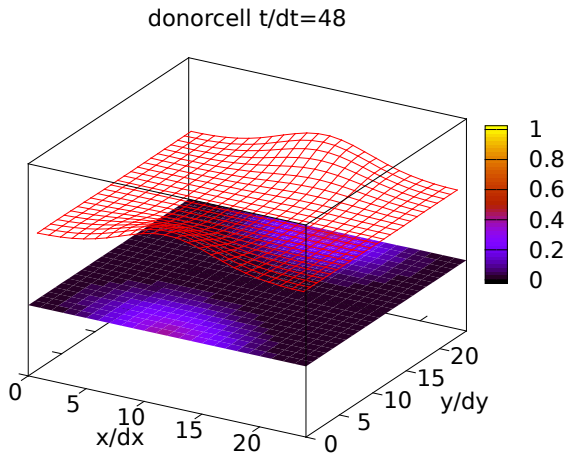

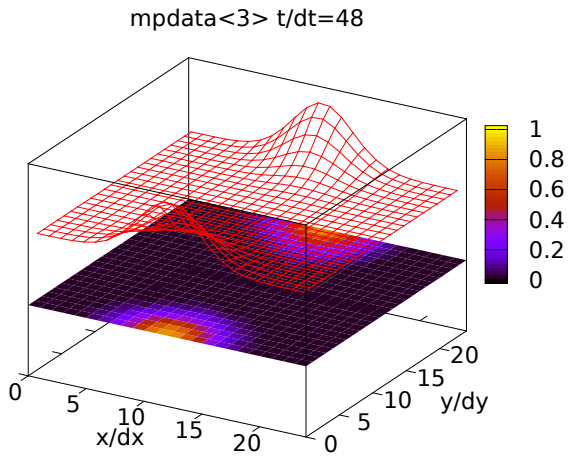

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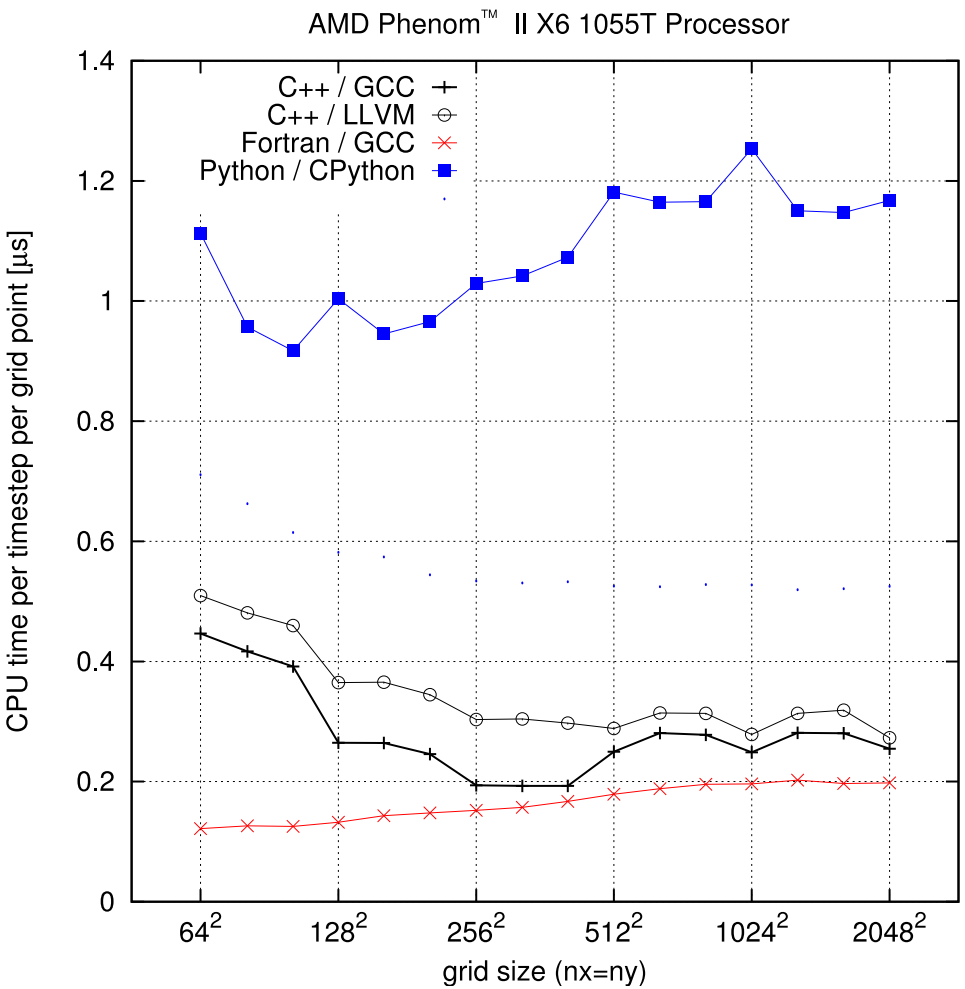

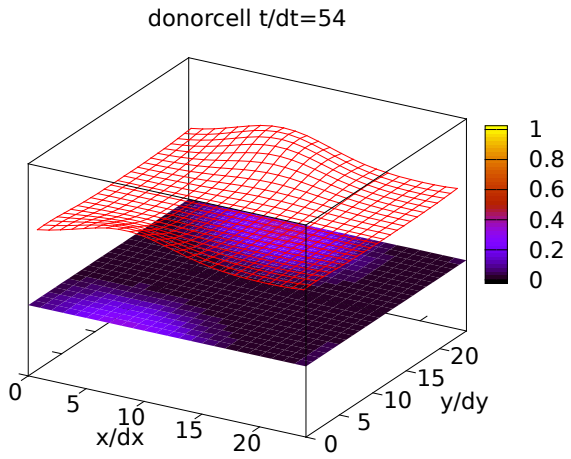

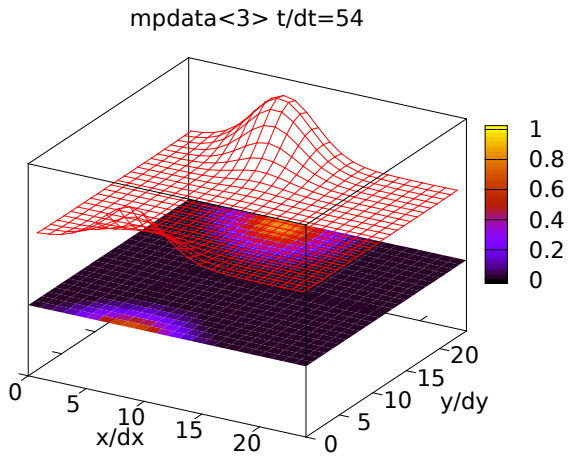

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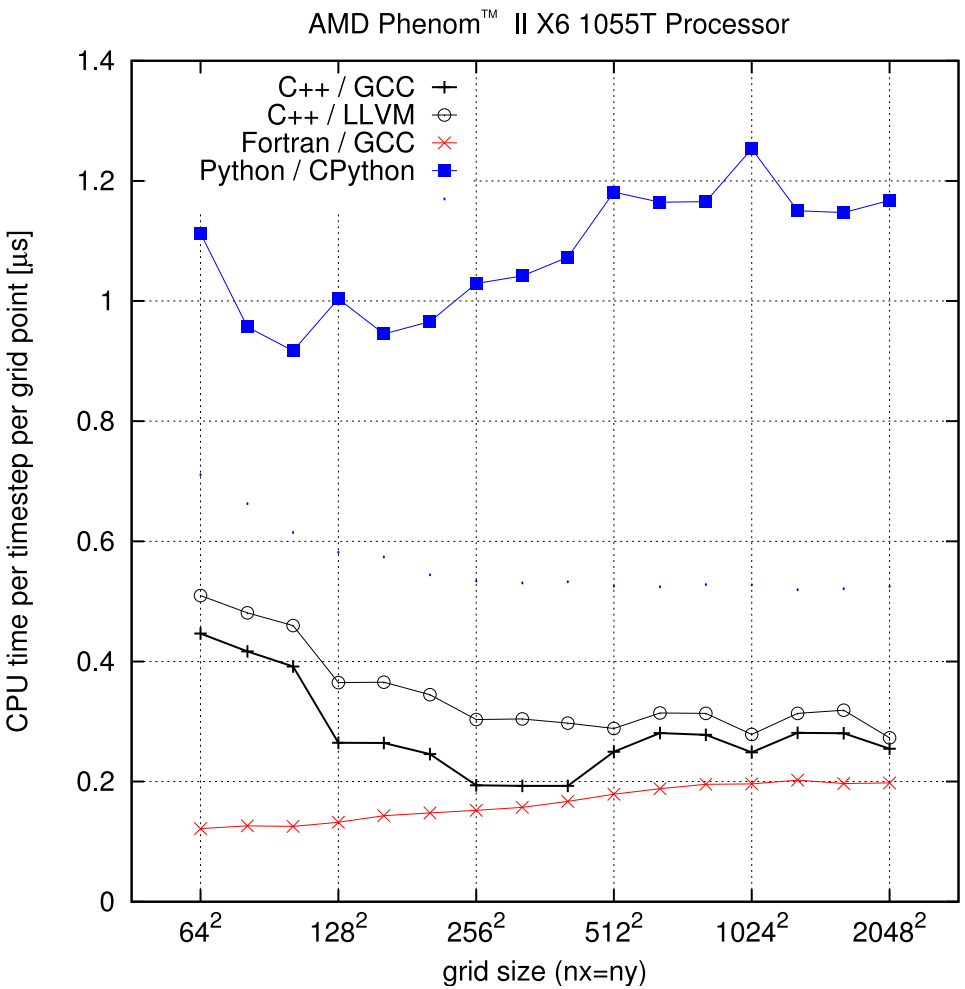

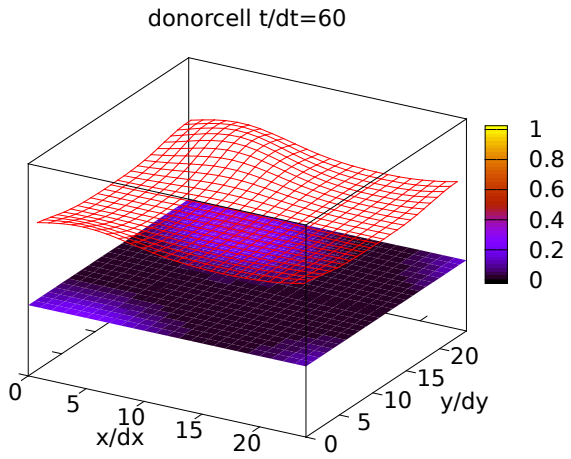

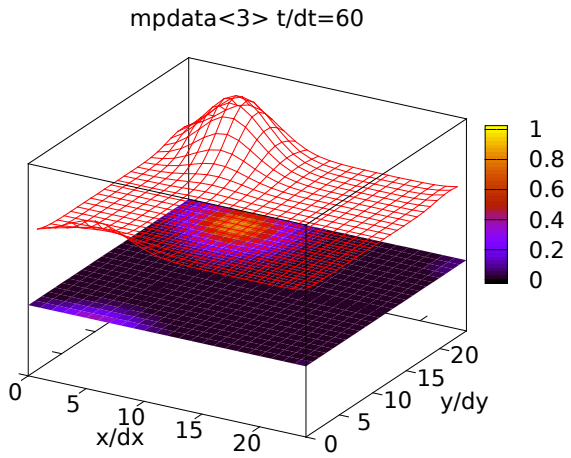

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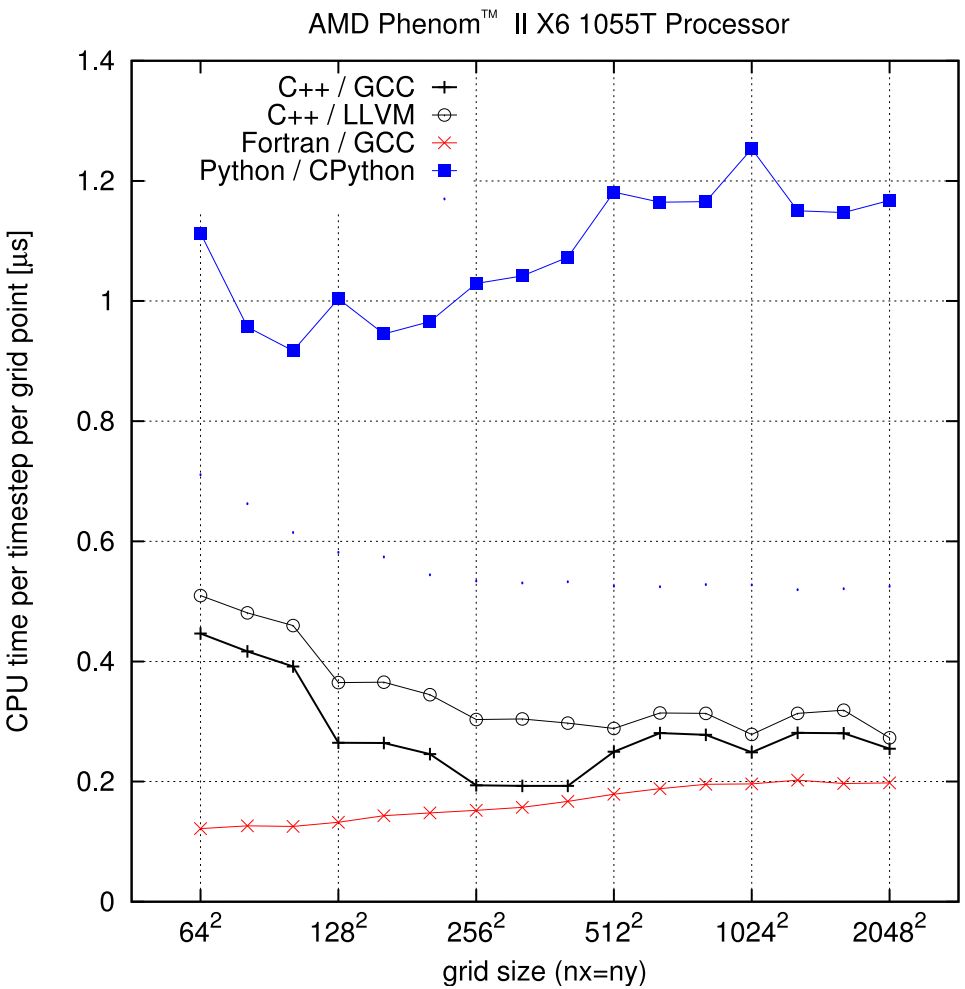

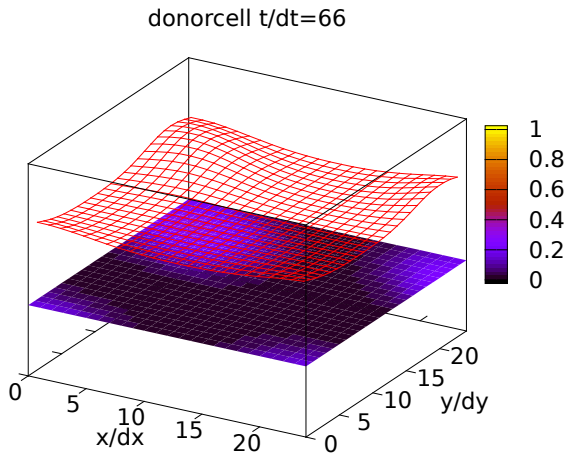

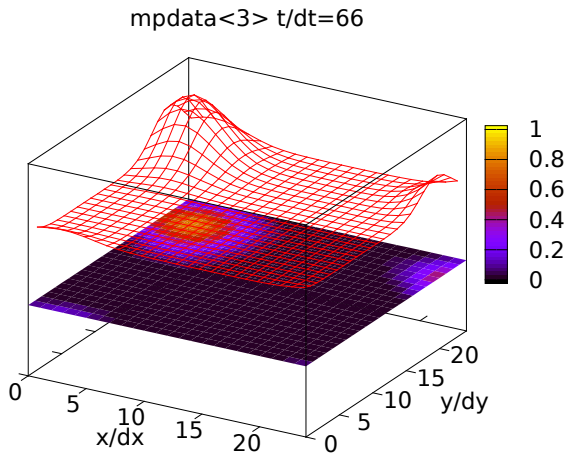

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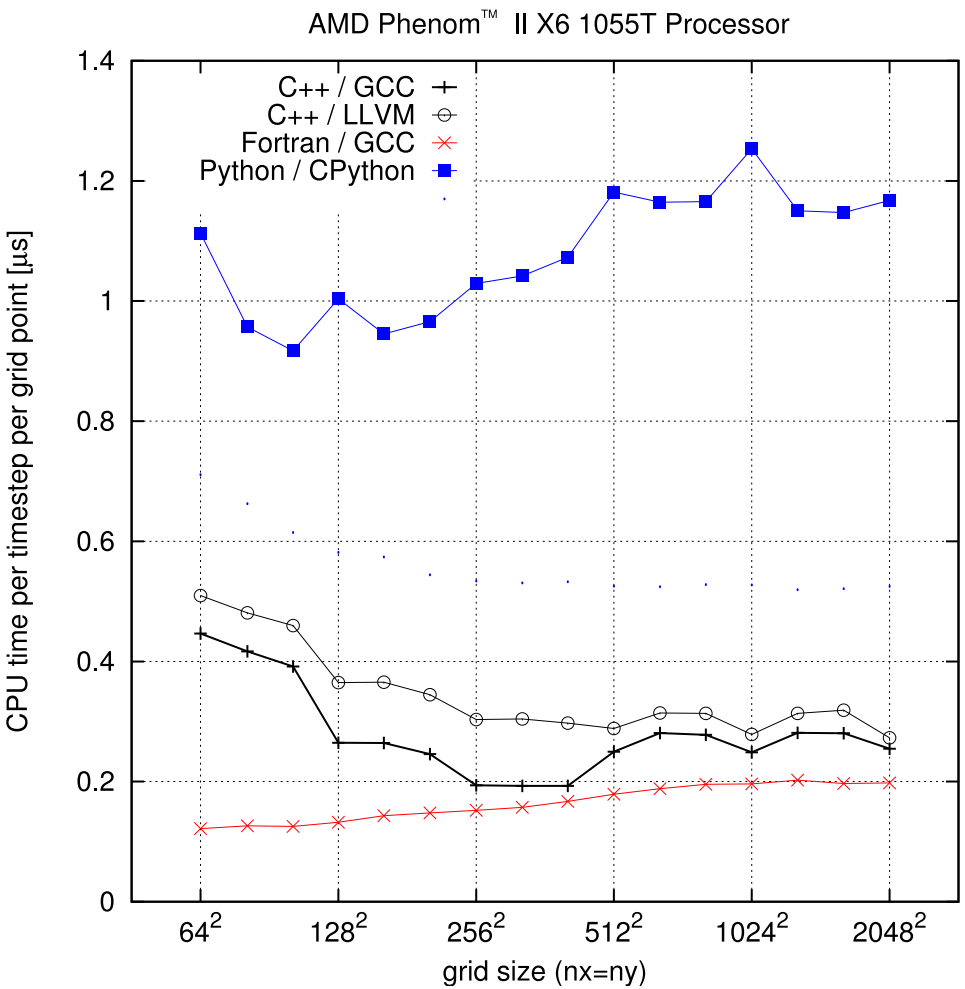

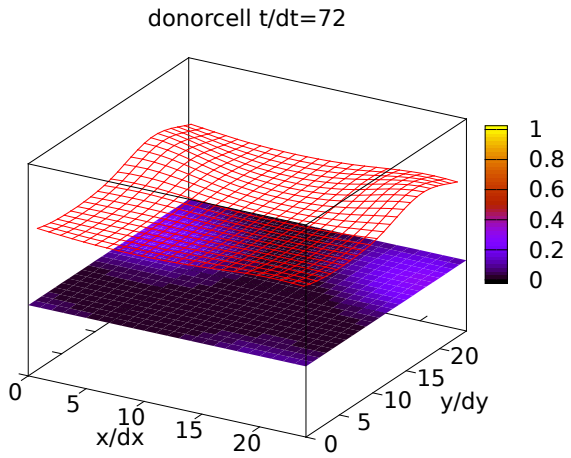

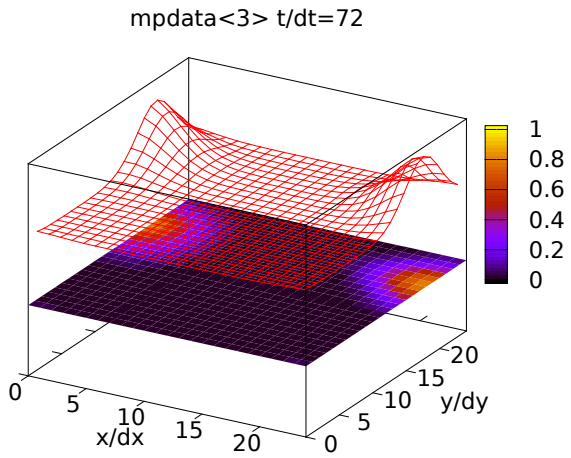

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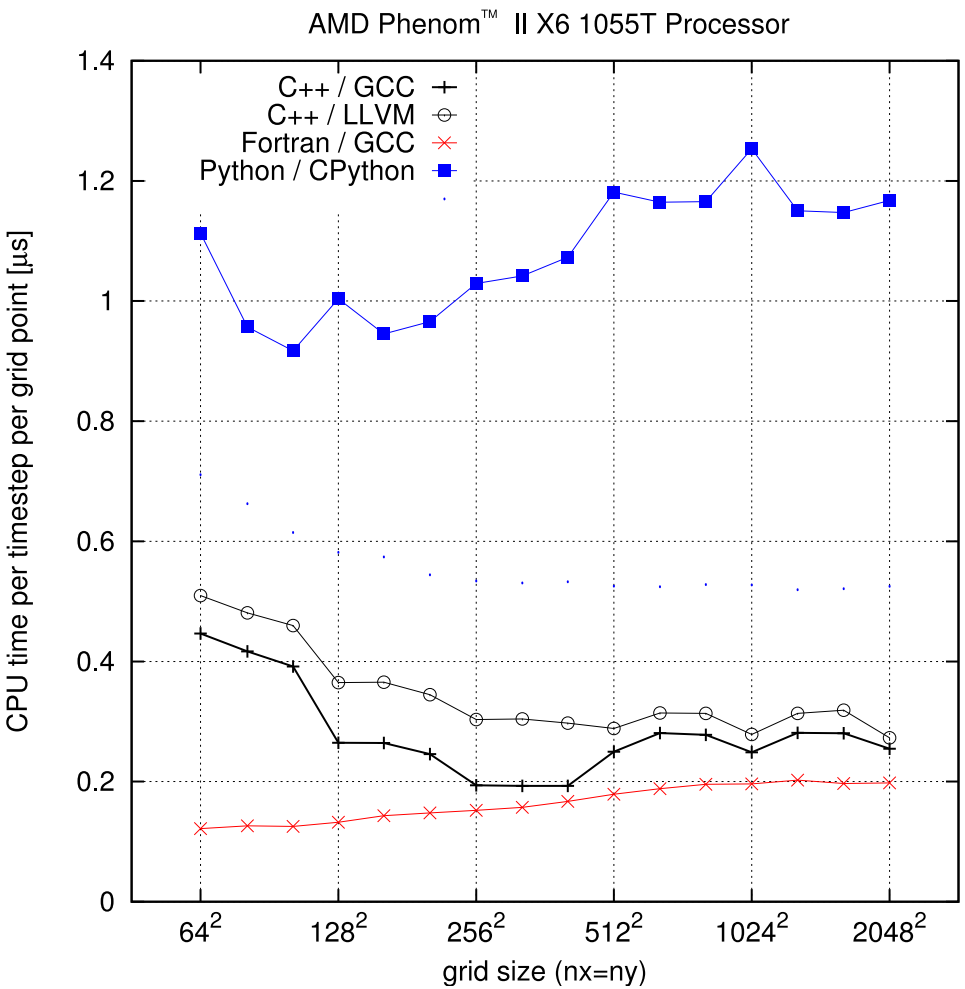

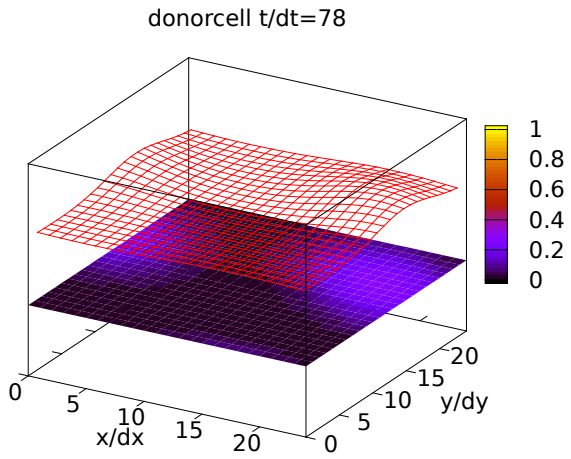

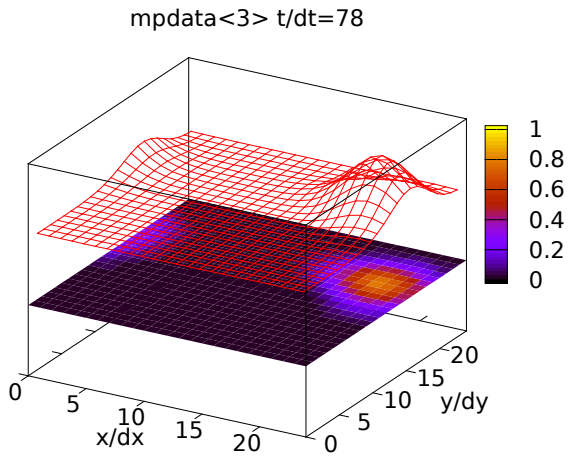

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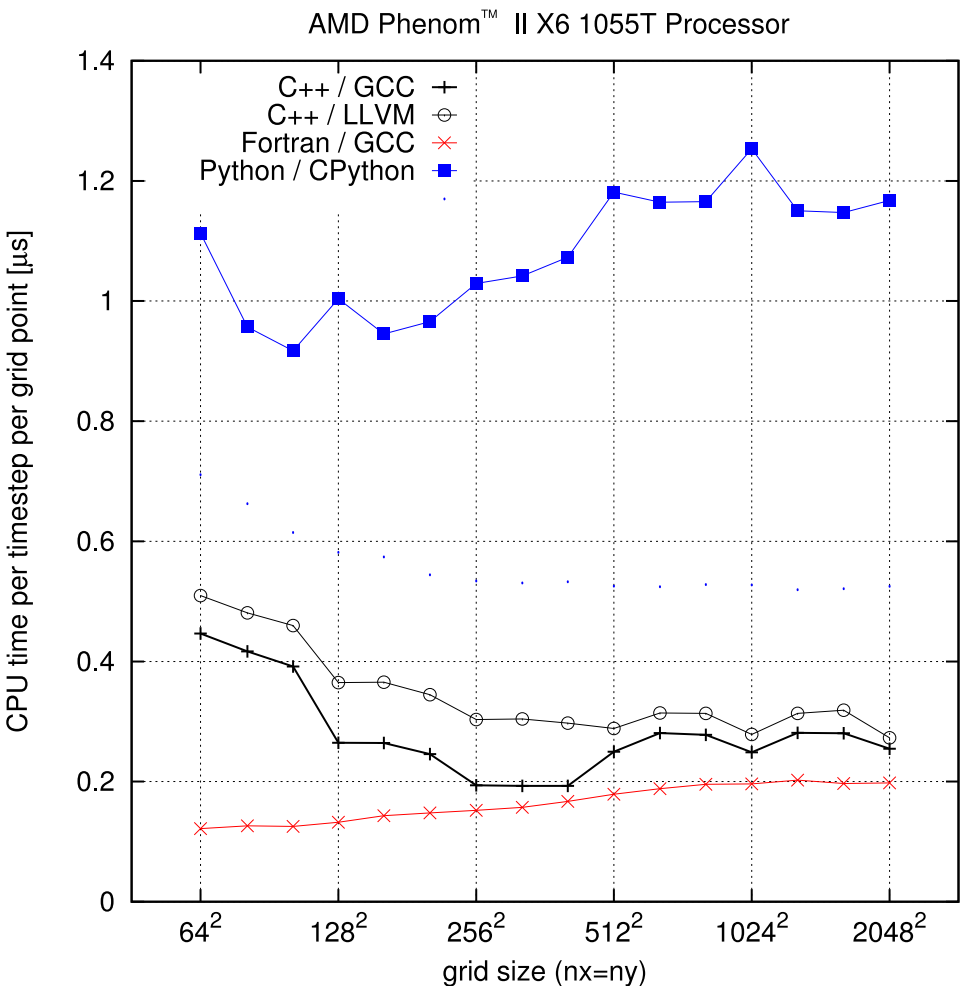

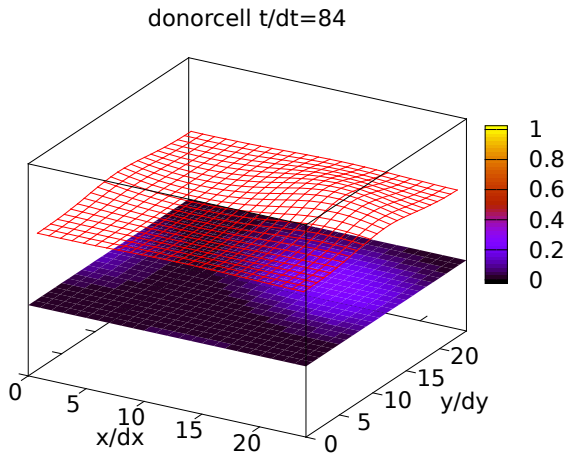

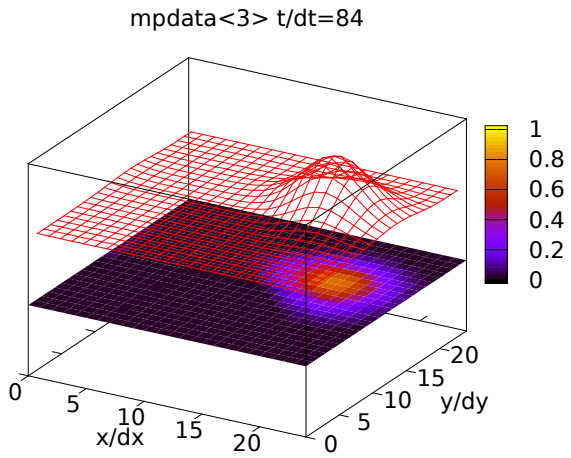

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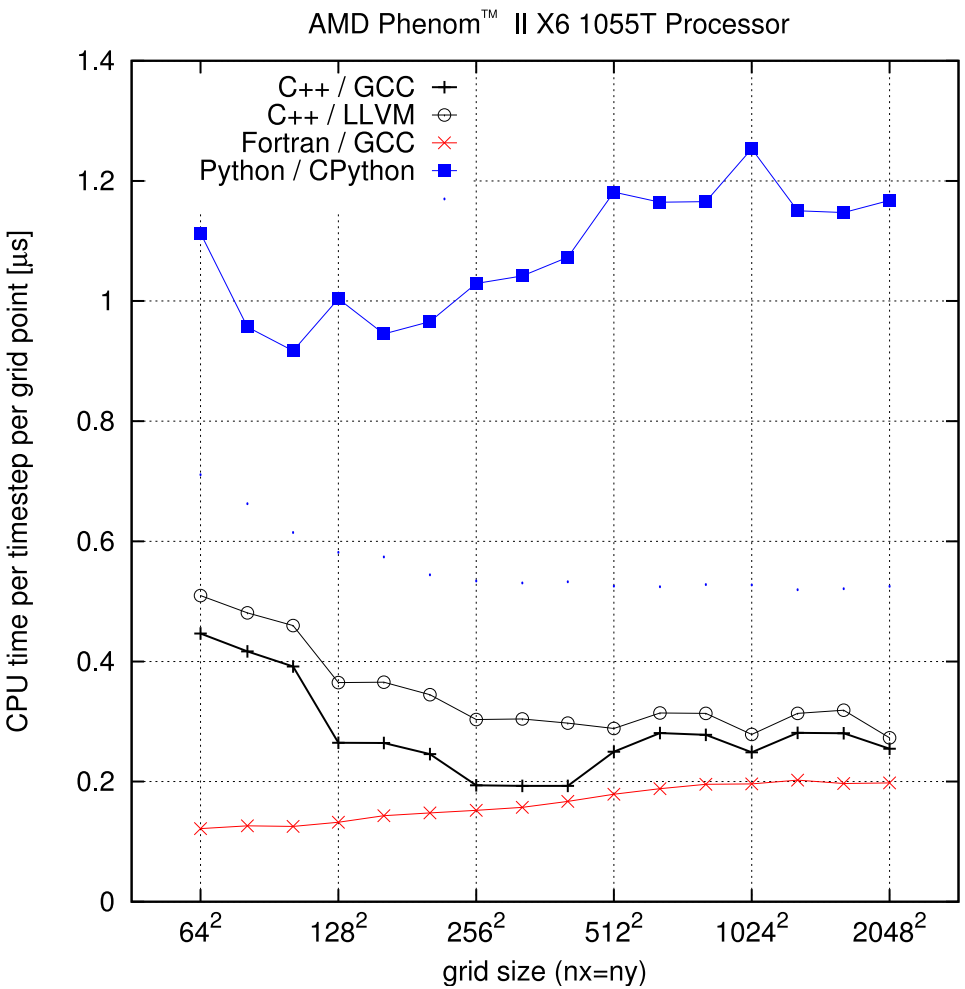

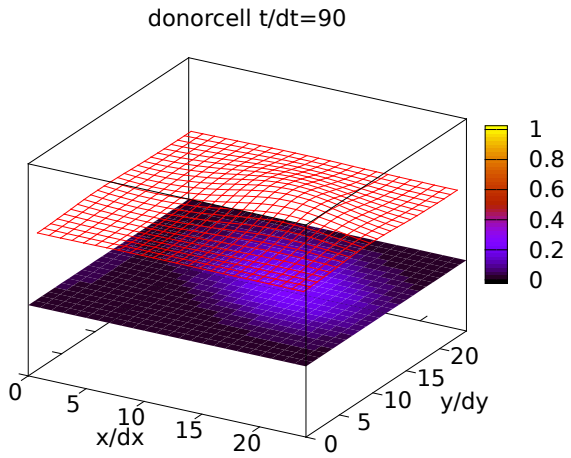

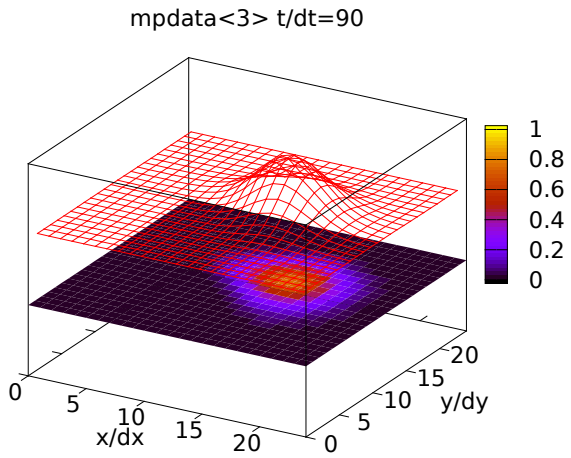

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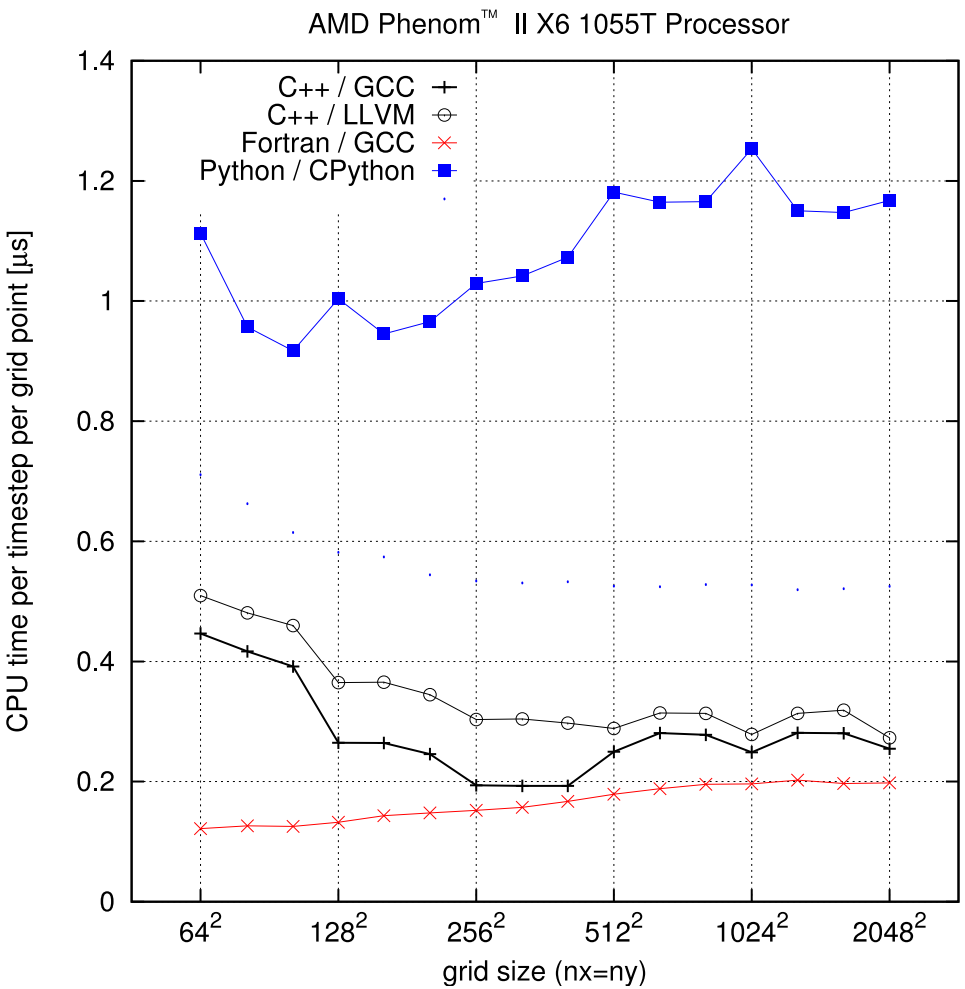

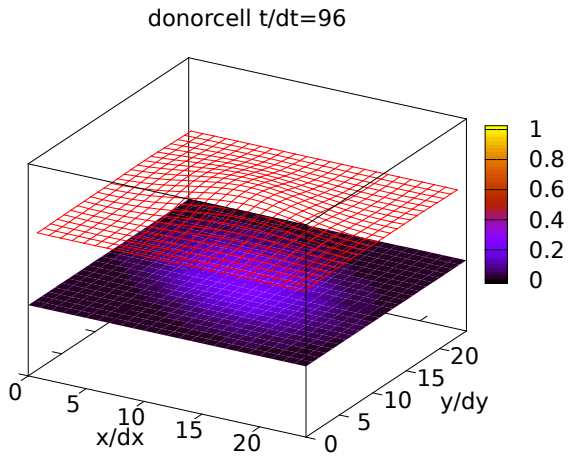

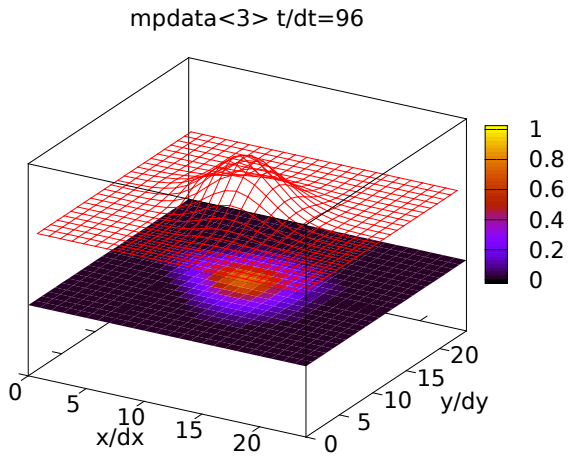

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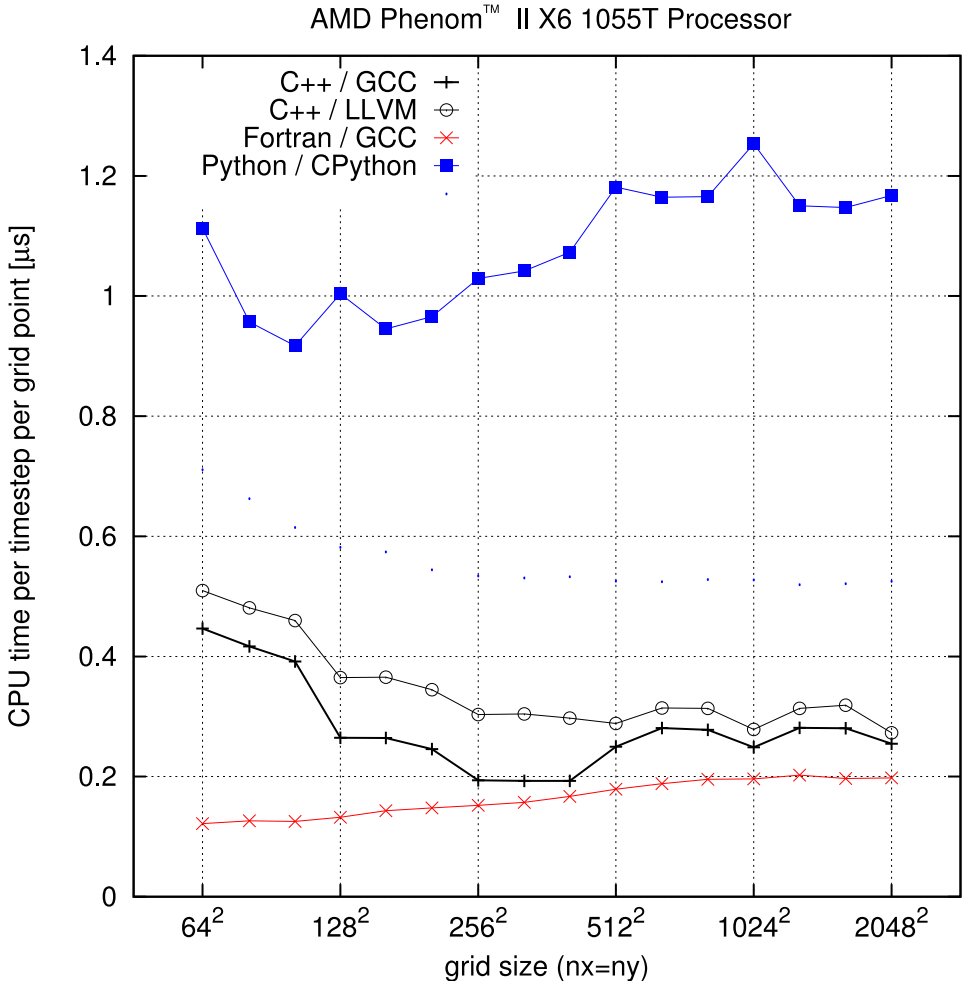

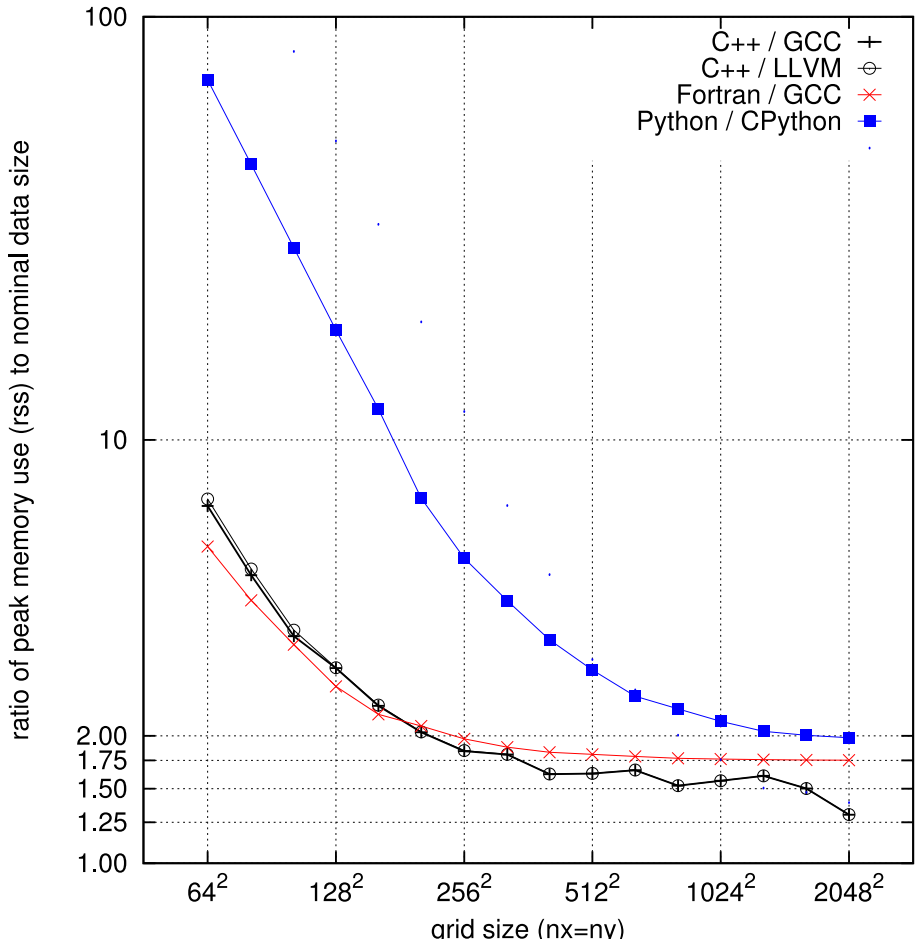

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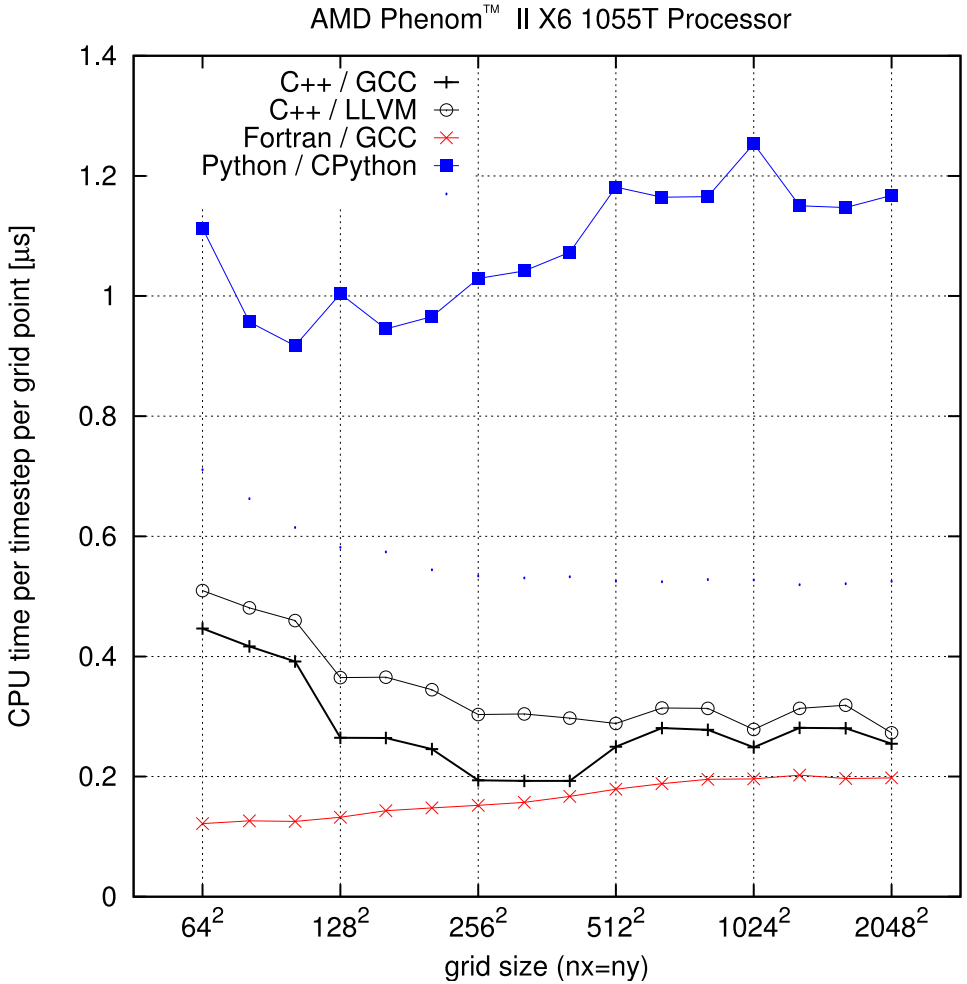

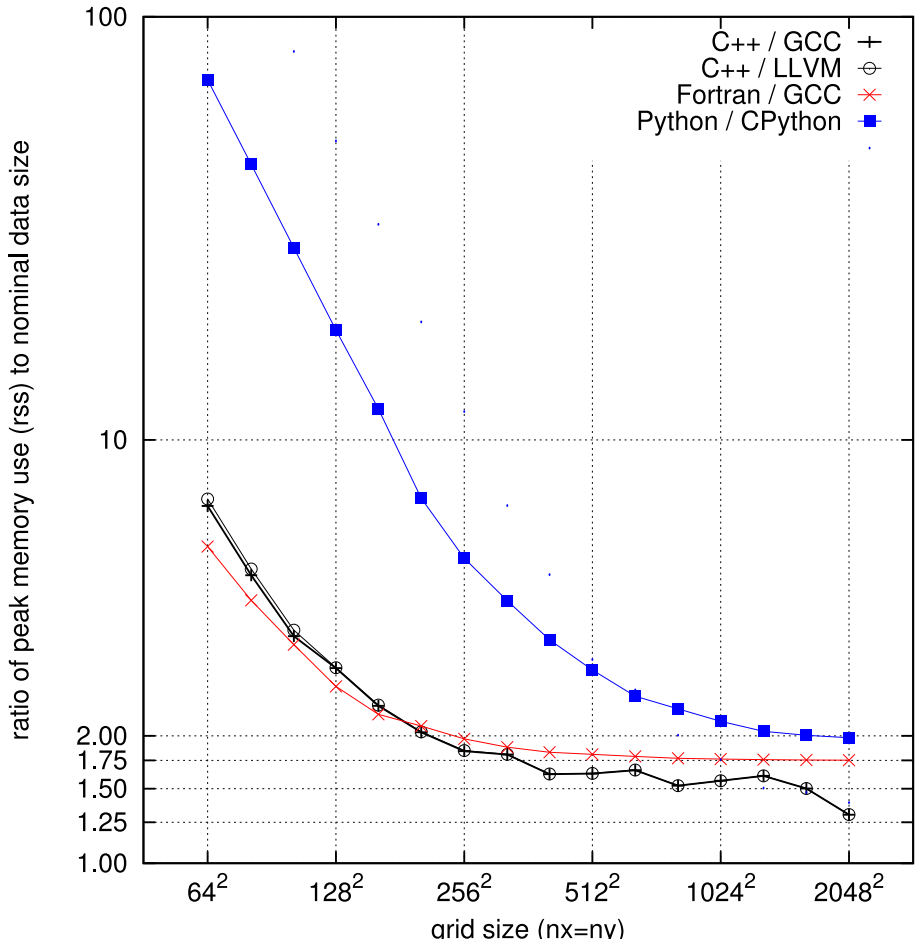

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  - alternative implementation of Python
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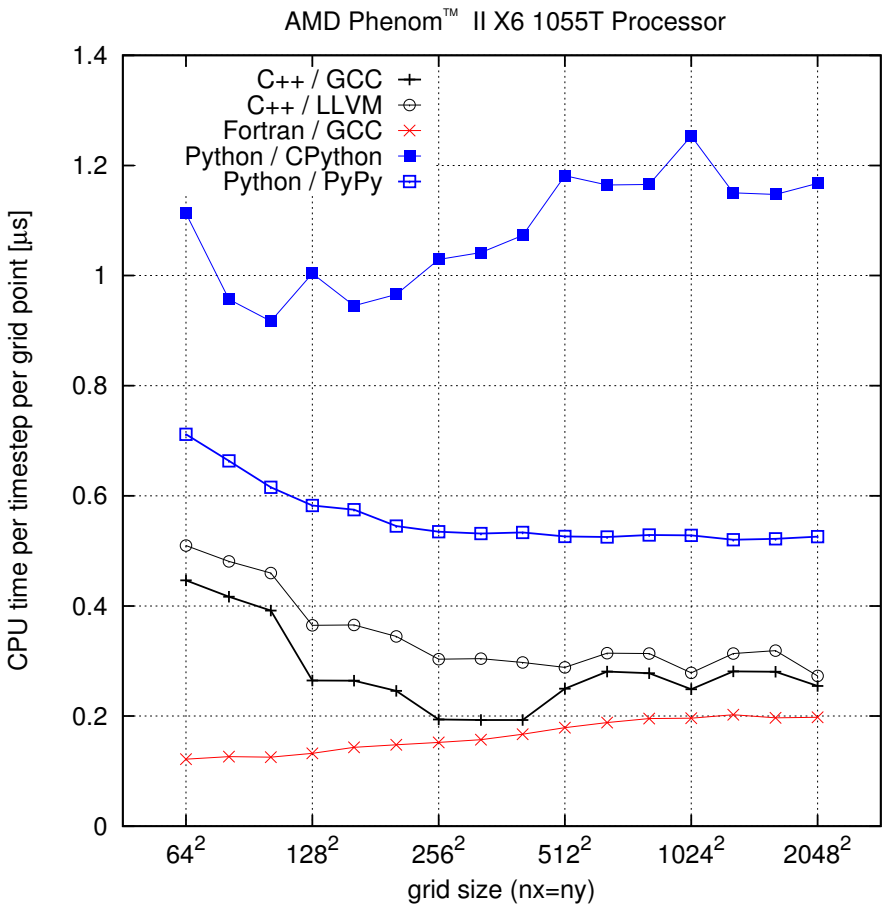

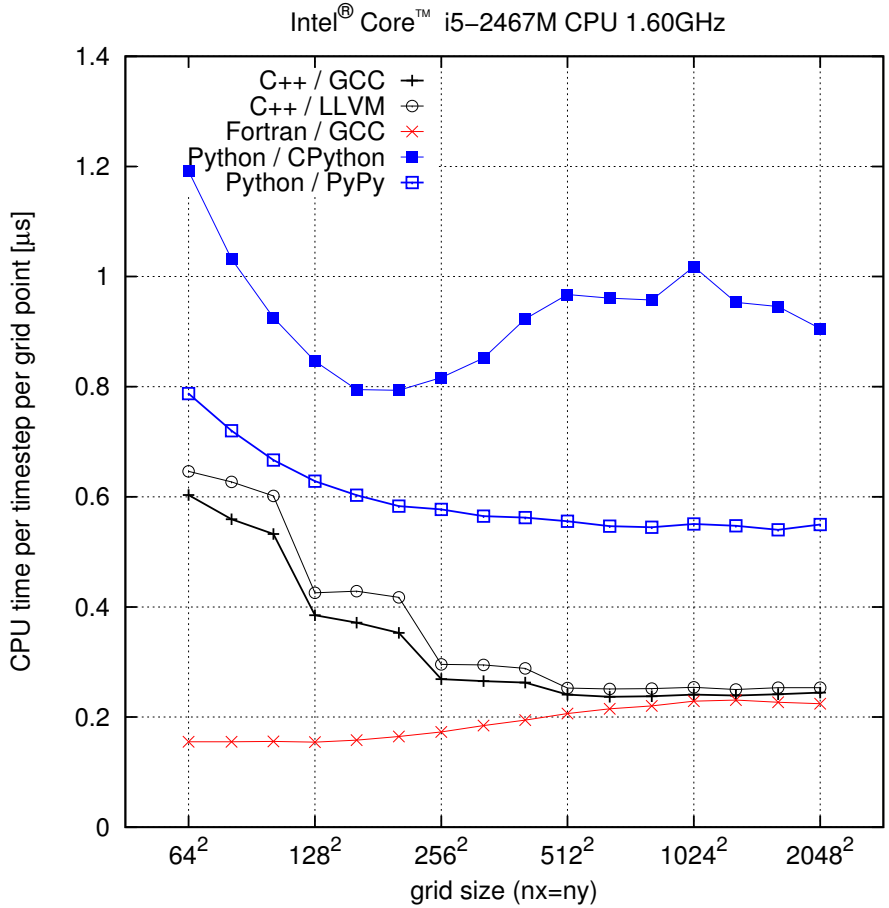

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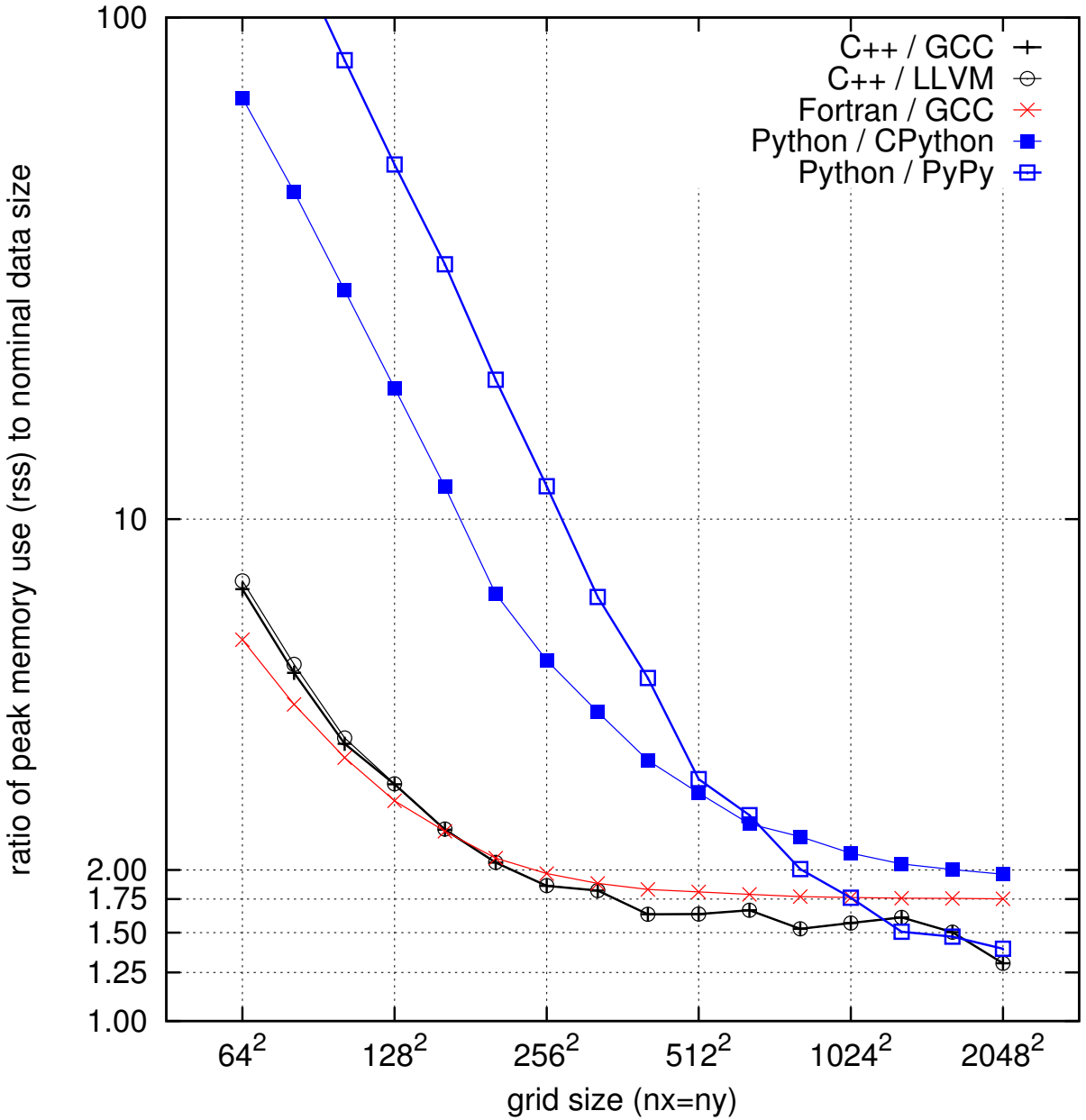

OOP numerics: language choice tradeoffs

capabilities for representing blackboard abstractions:

- C++, Python and Fortran provide comparable functionalities for compact representation of mathematical abstractions thanks to:
  - loop-free array arithmetics
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  - indirections allowing permuting array indices
  - fractional indexing through operator overloading
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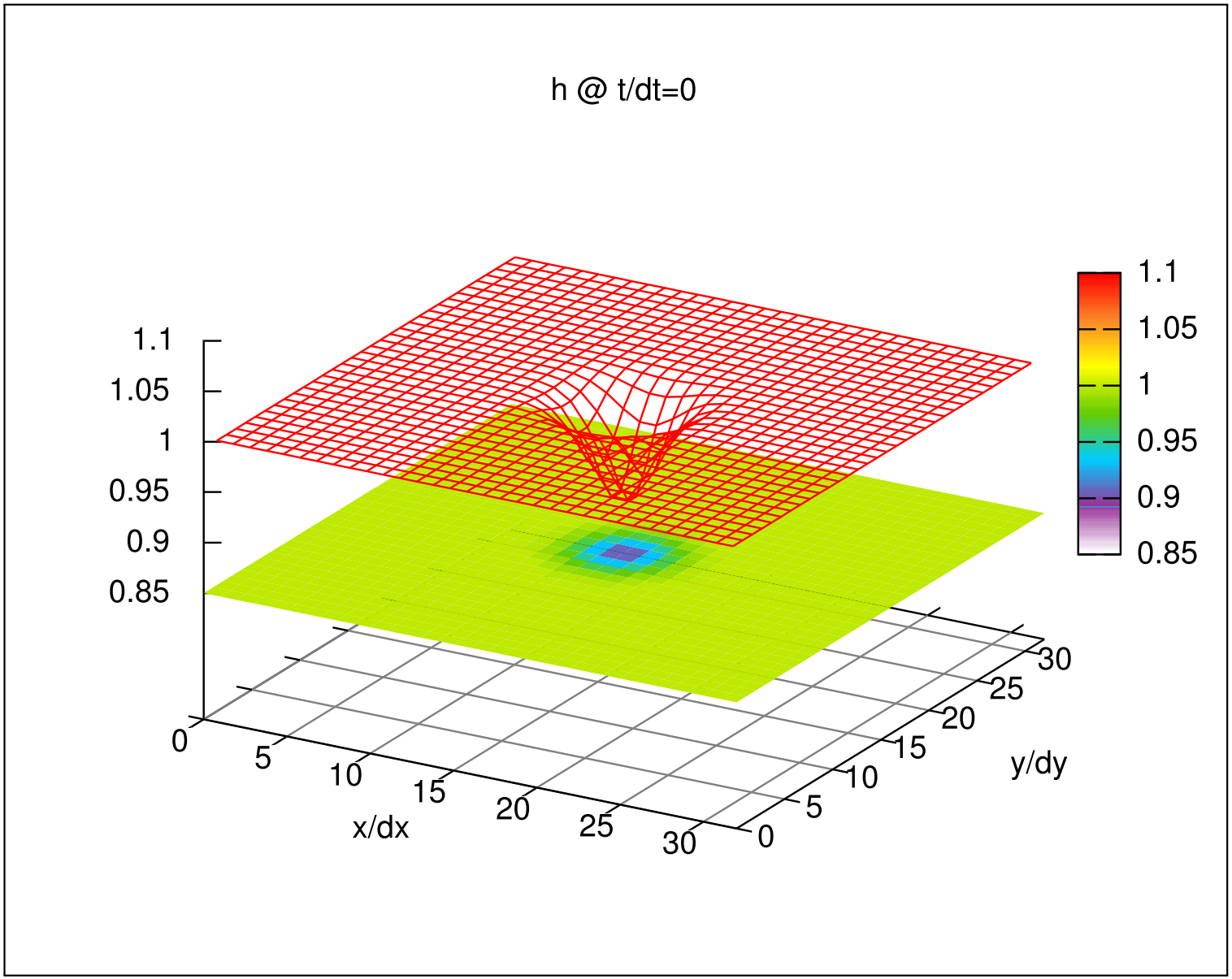

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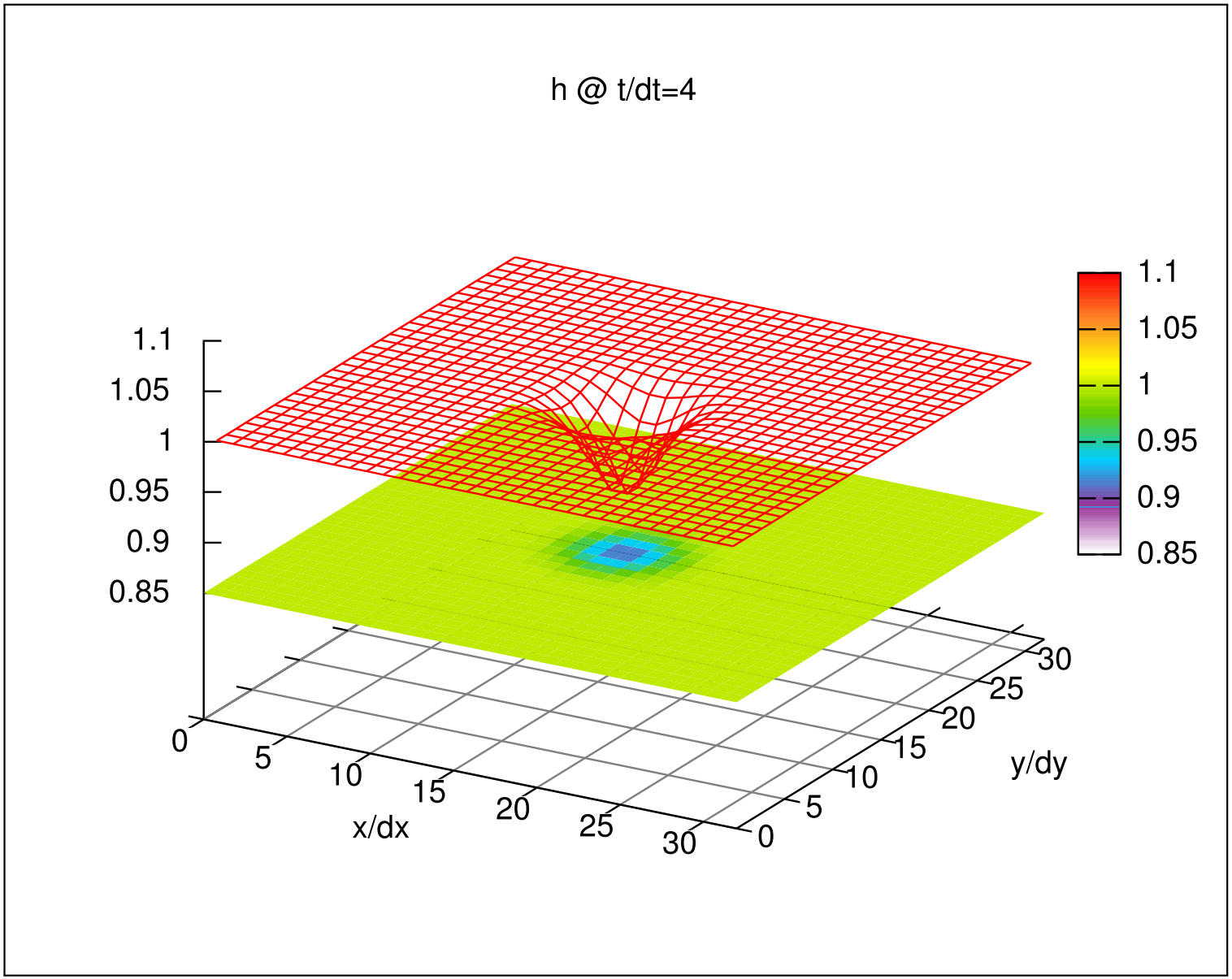

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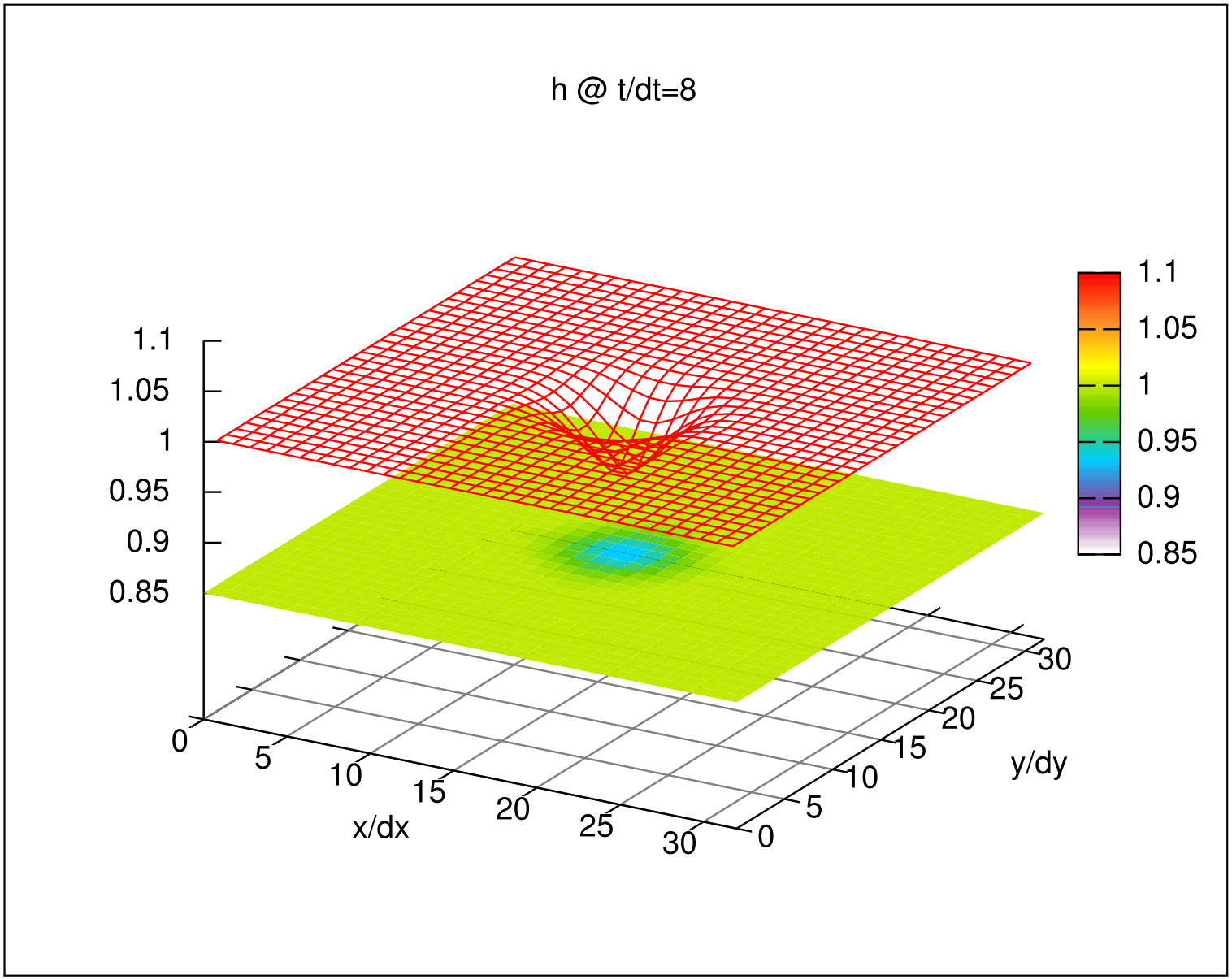

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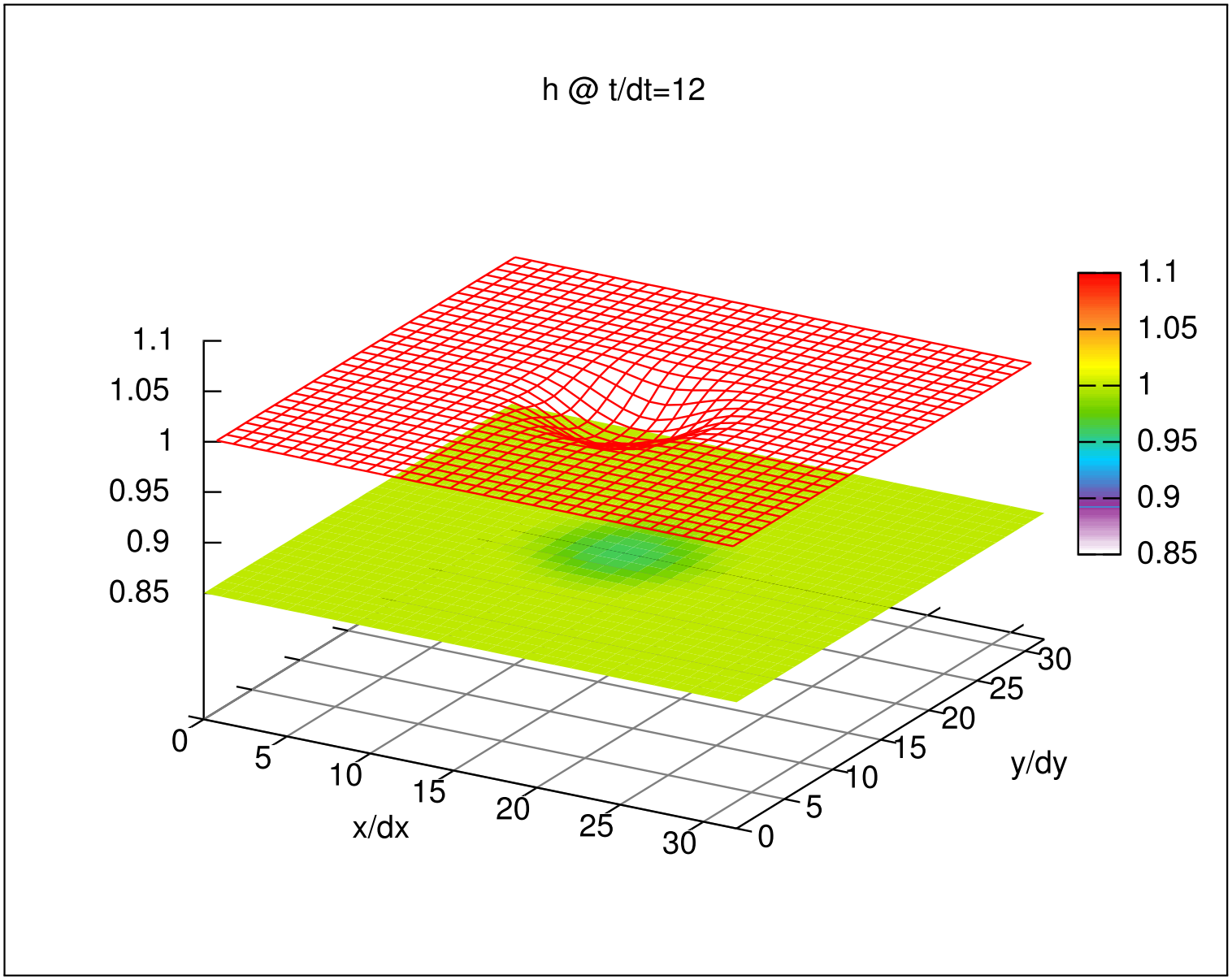

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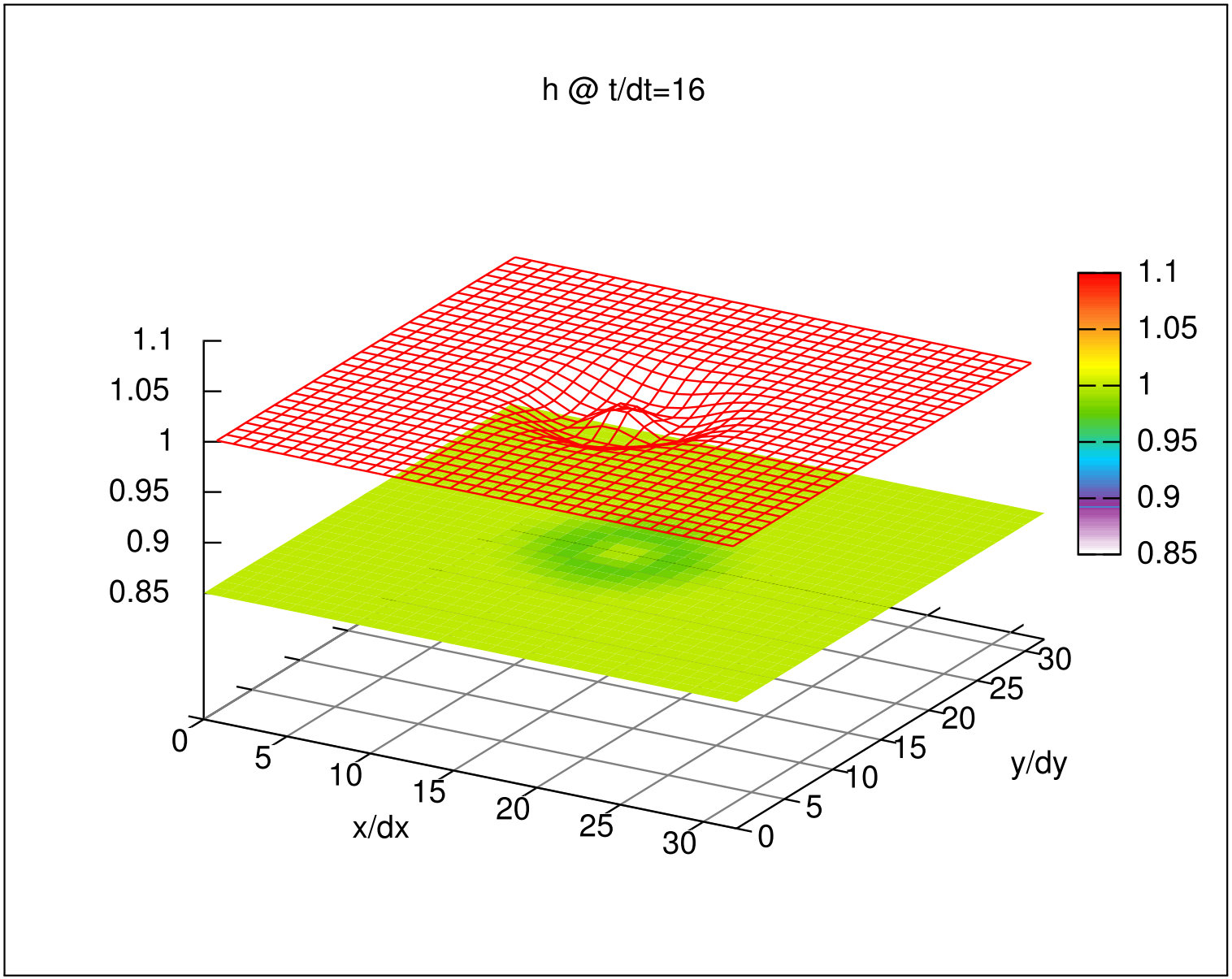

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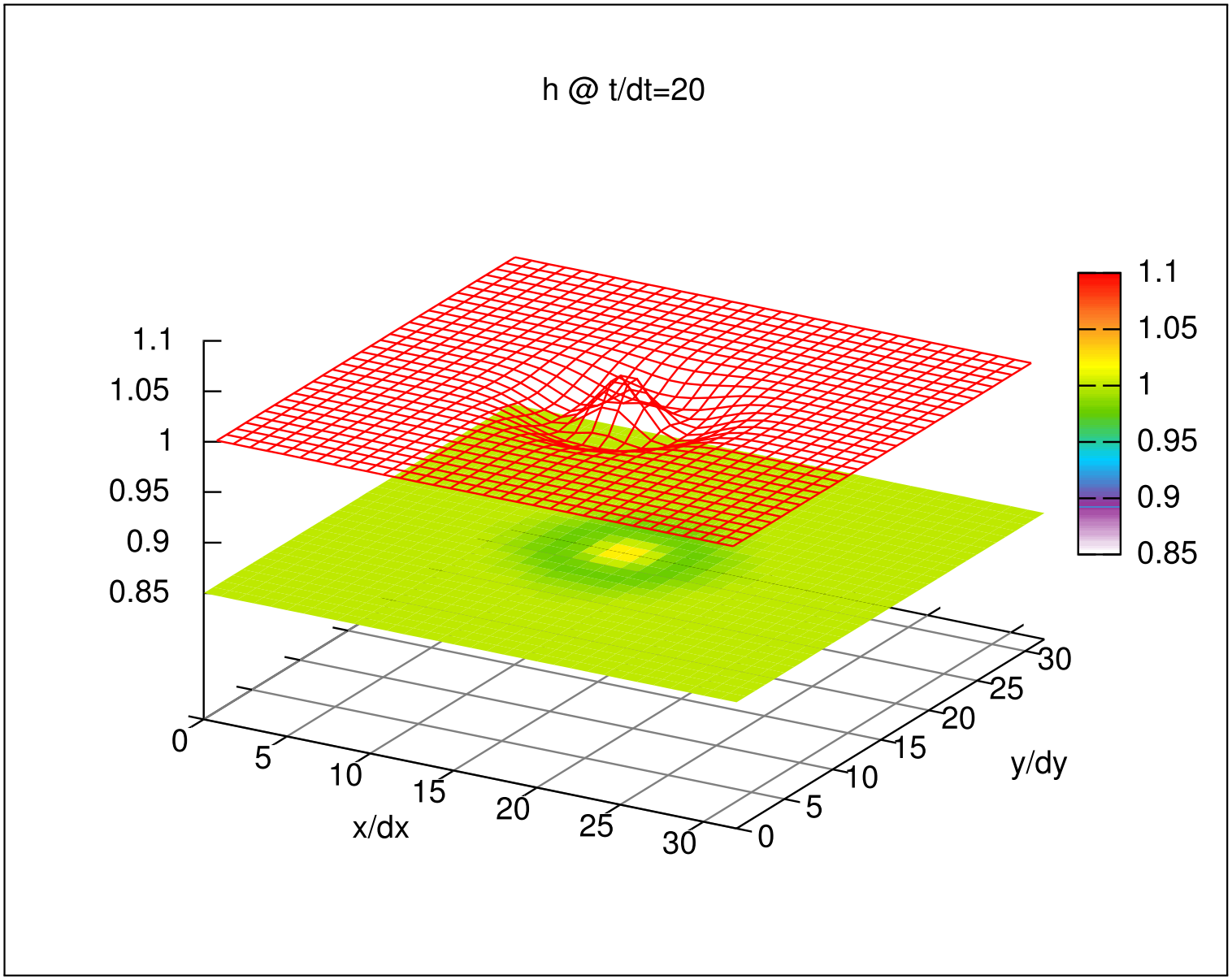

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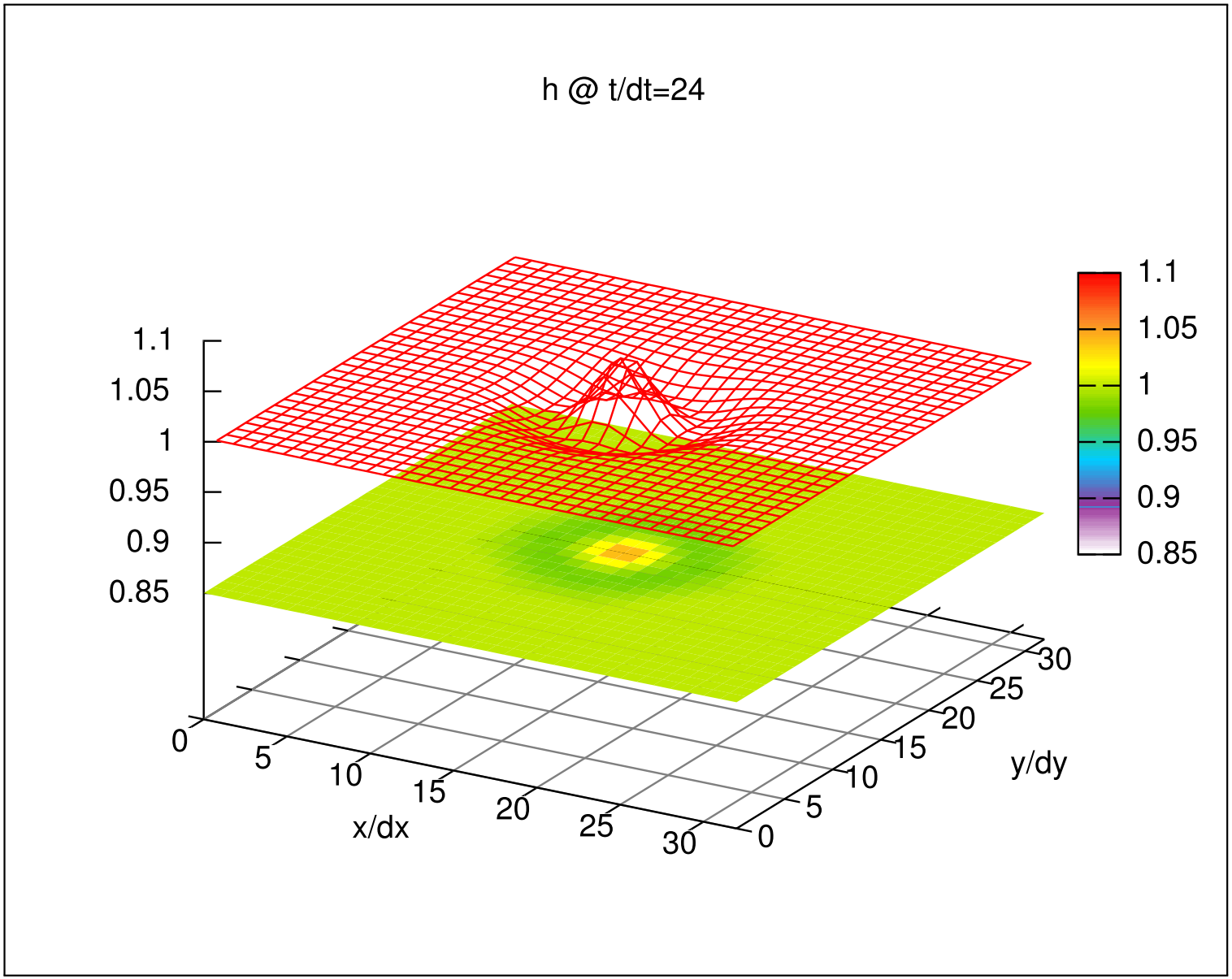

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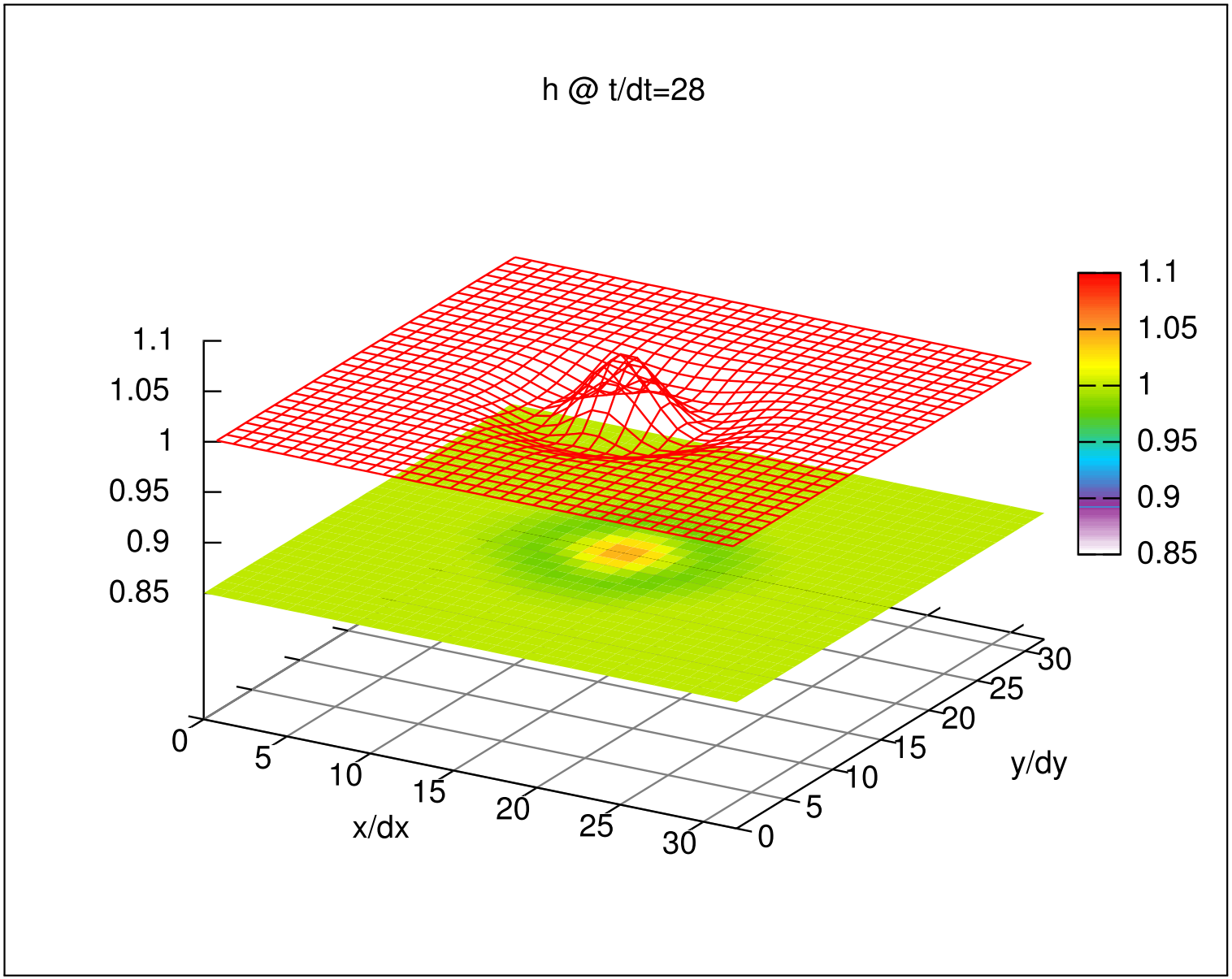

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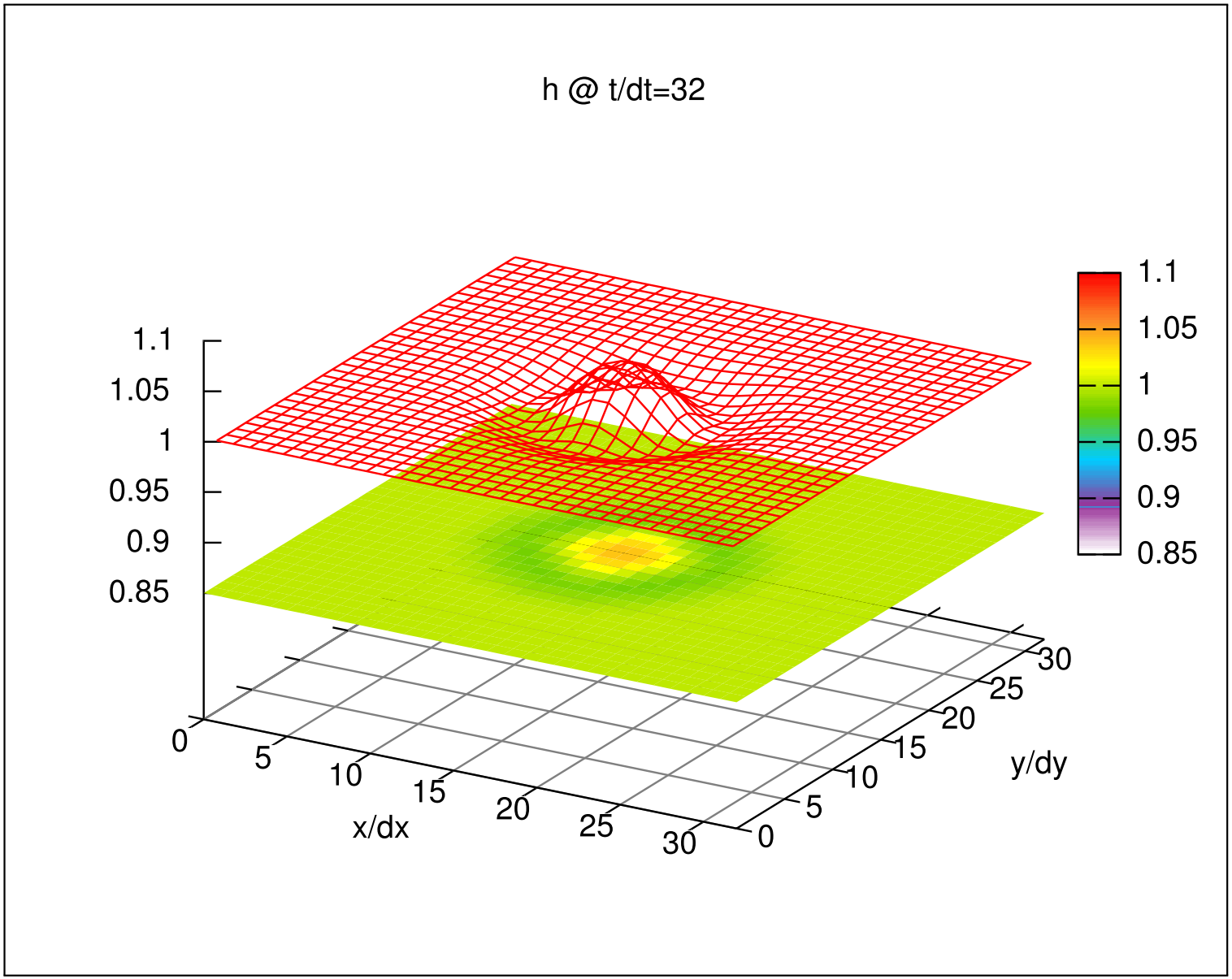

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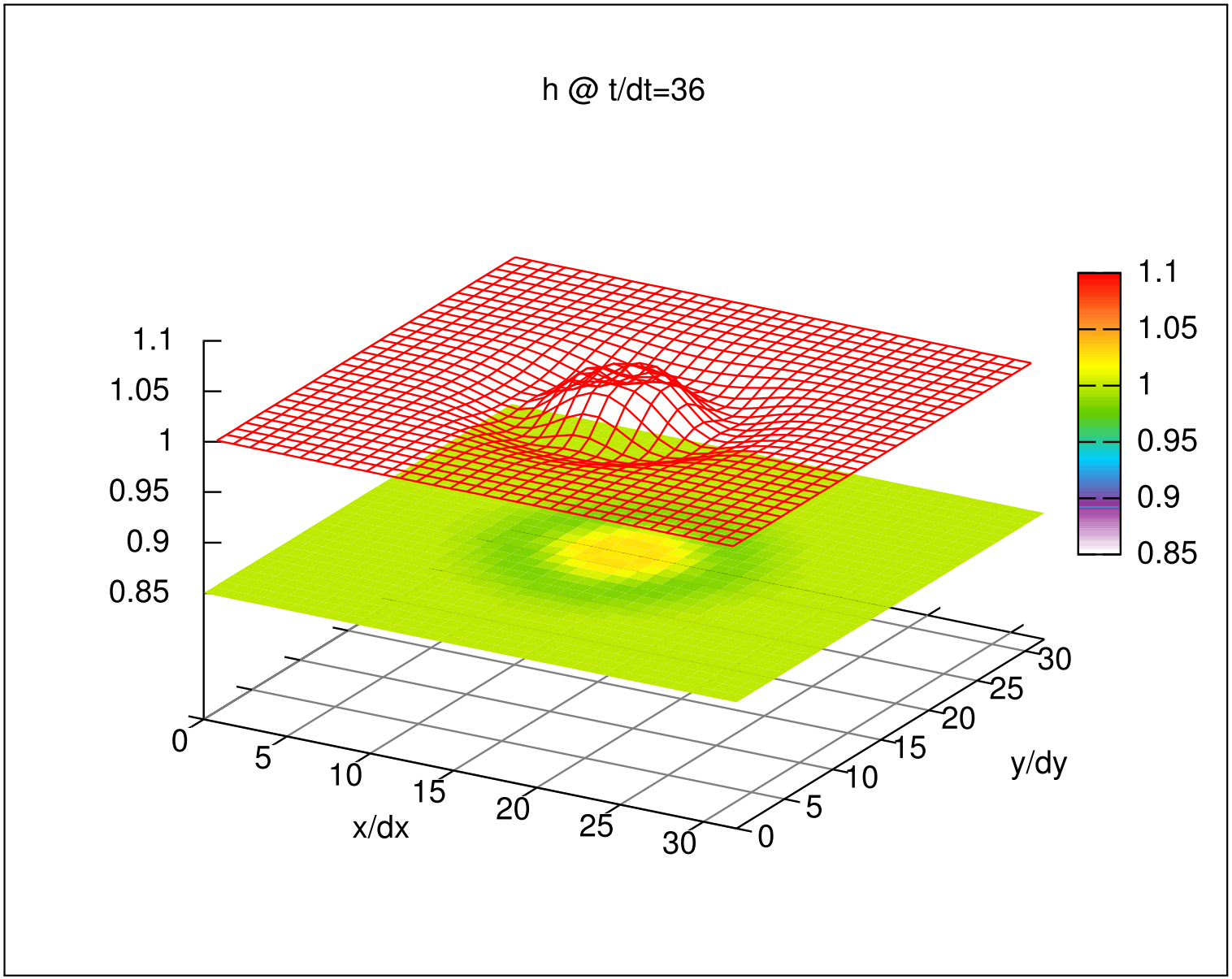

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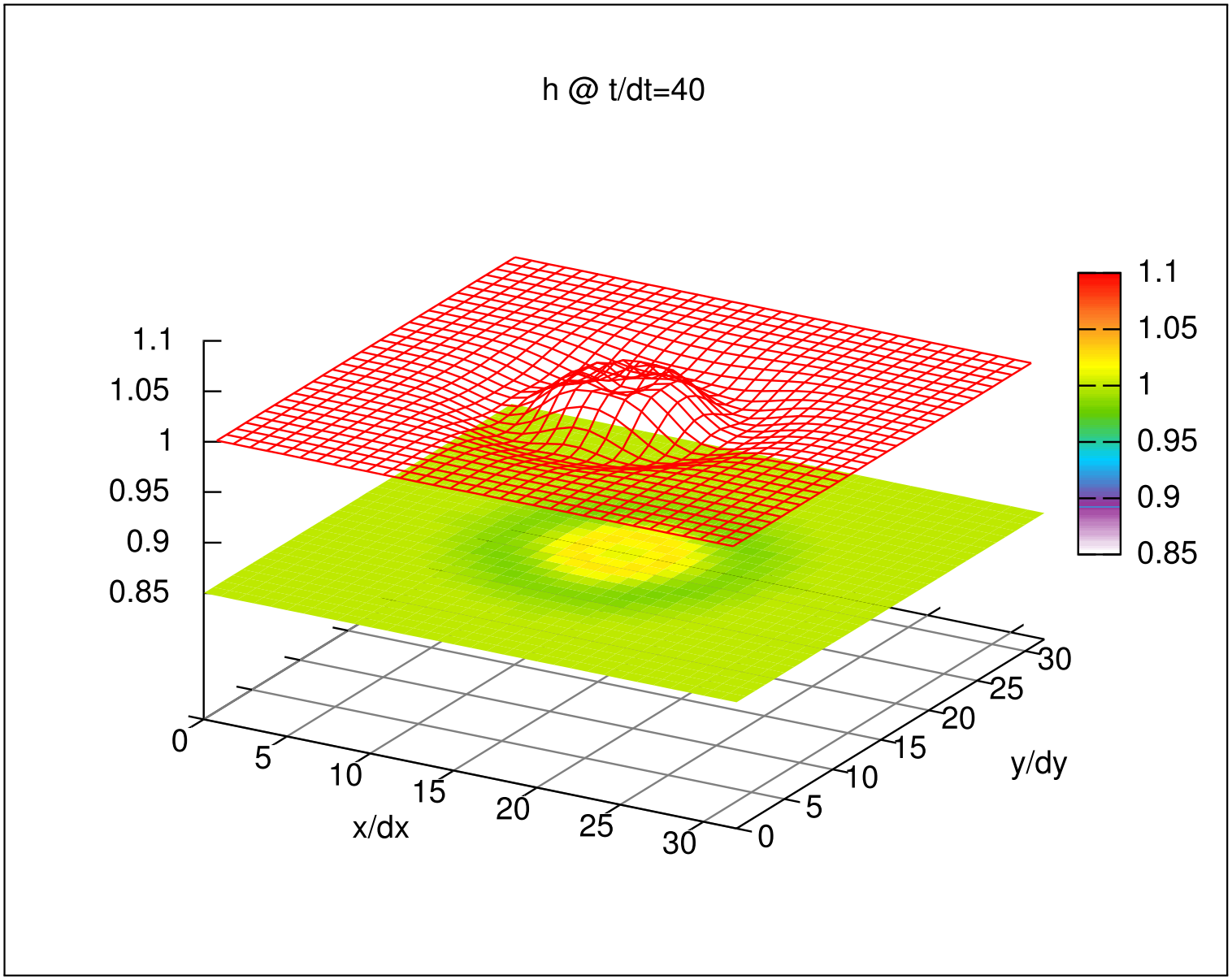

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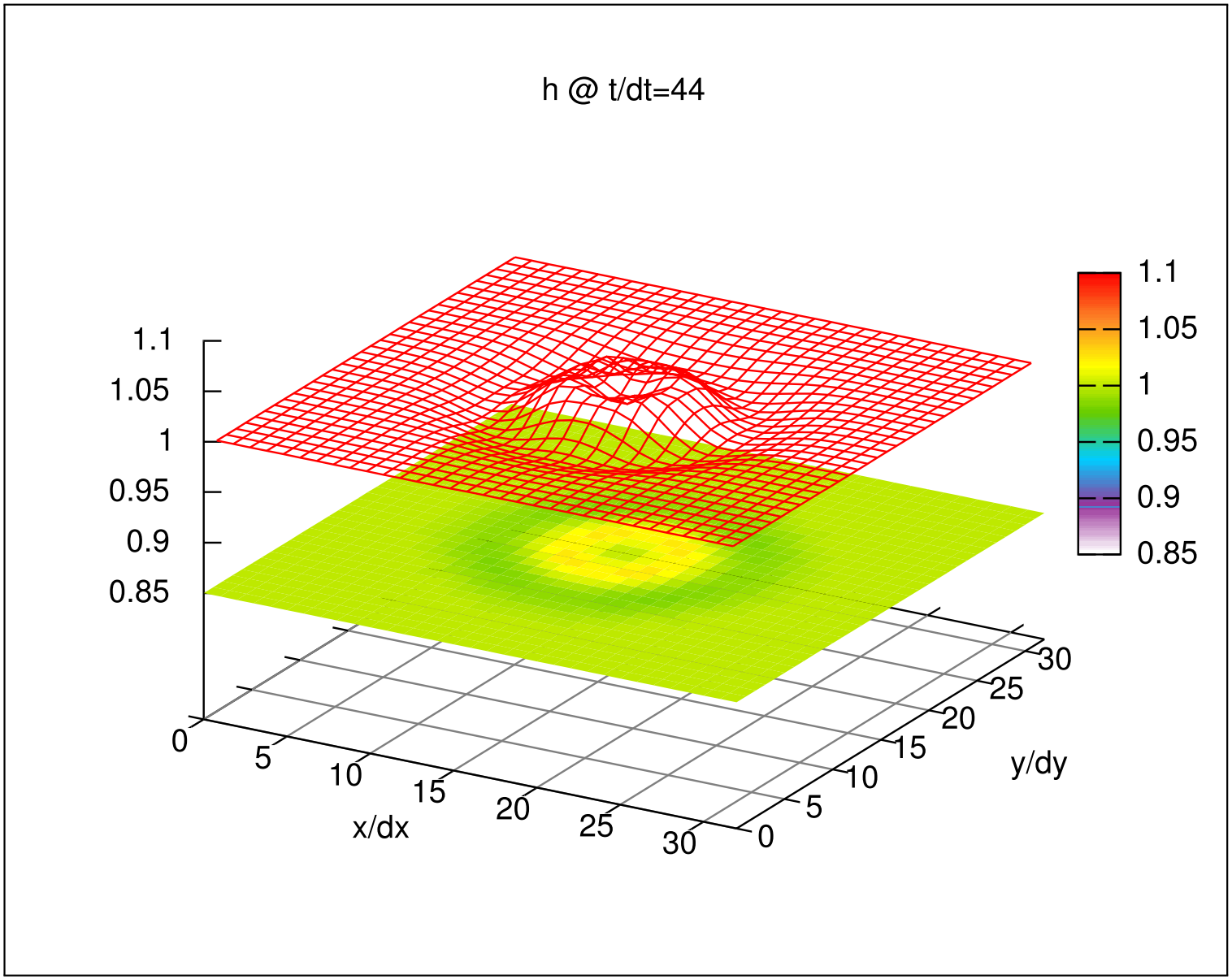

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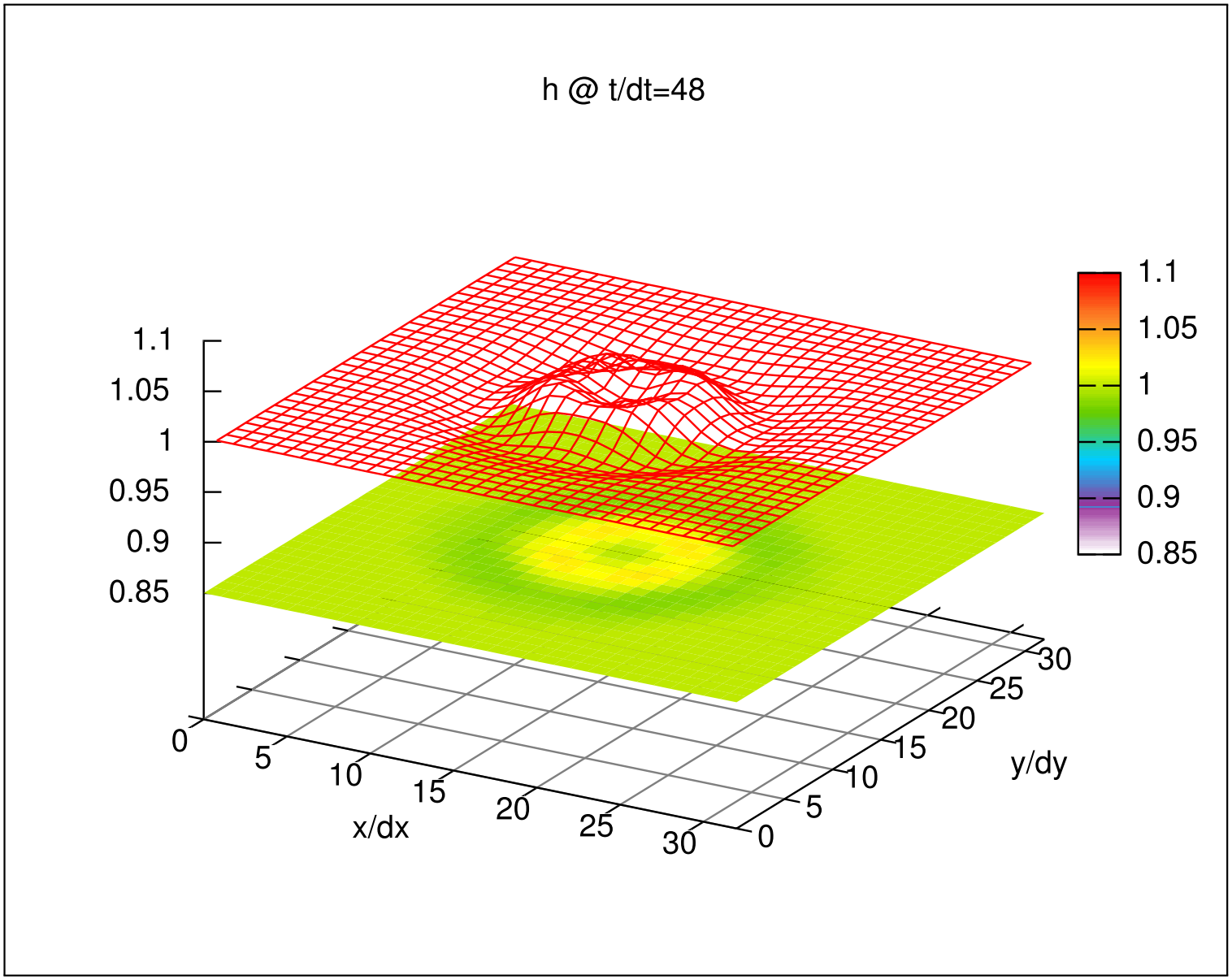

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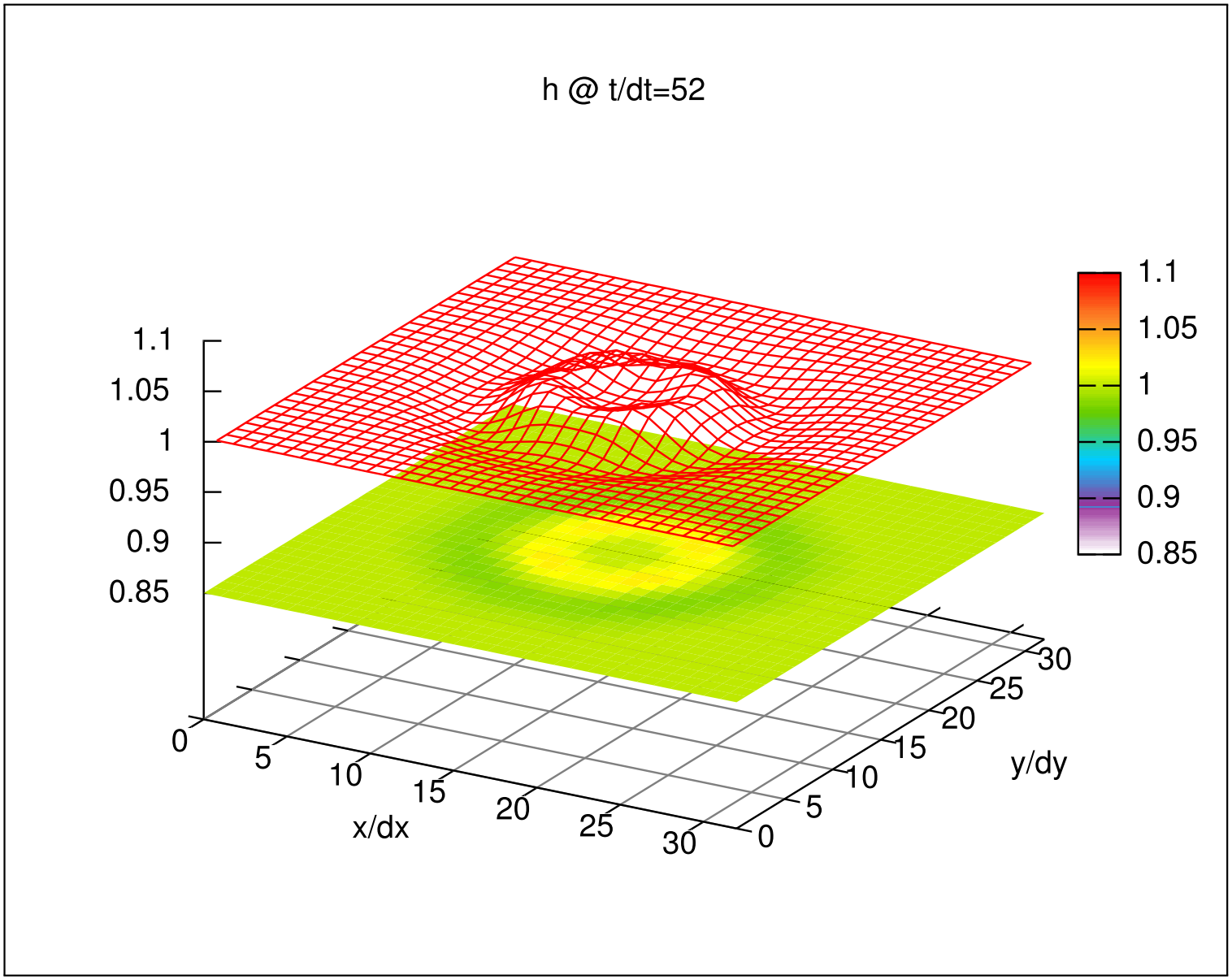

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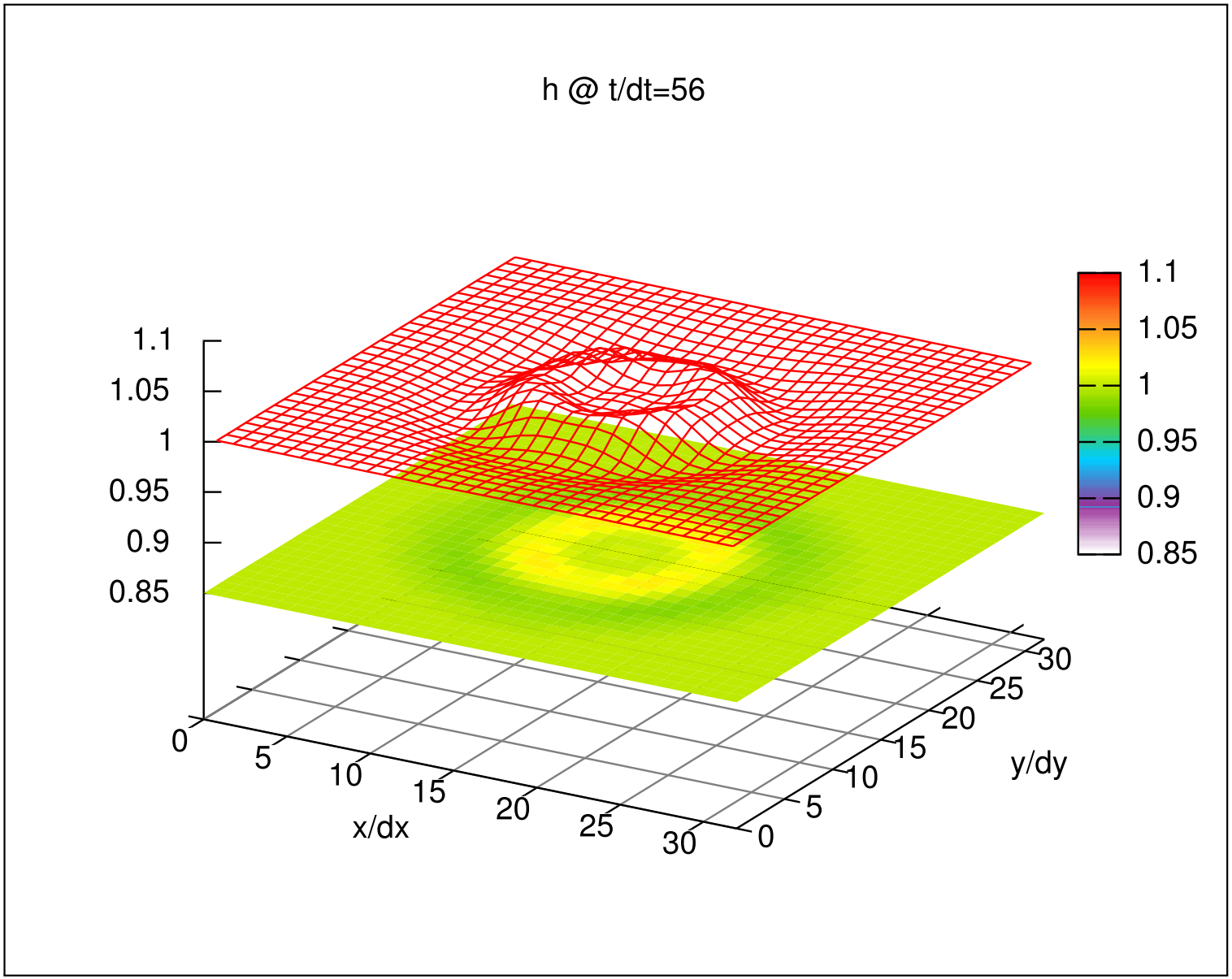

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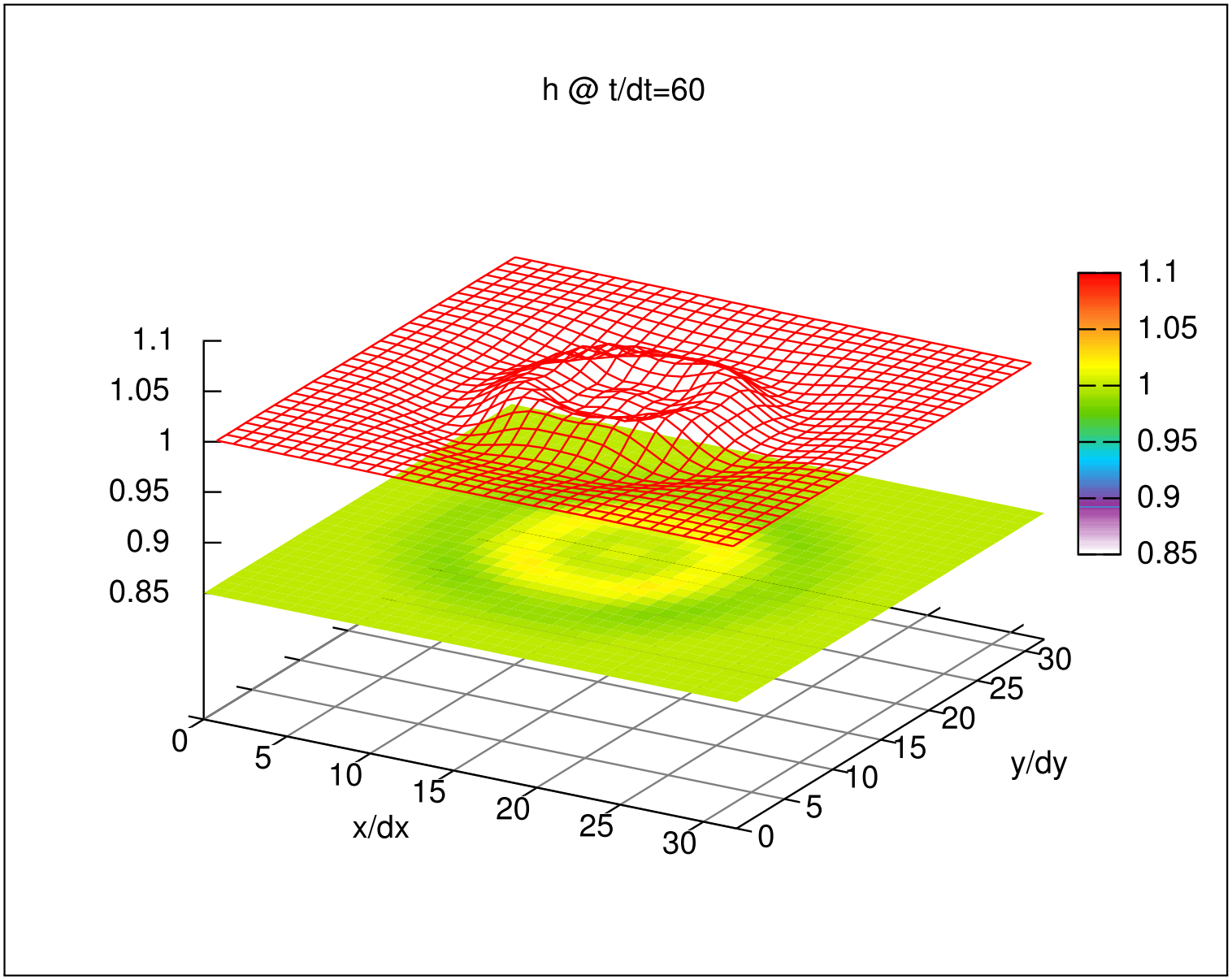

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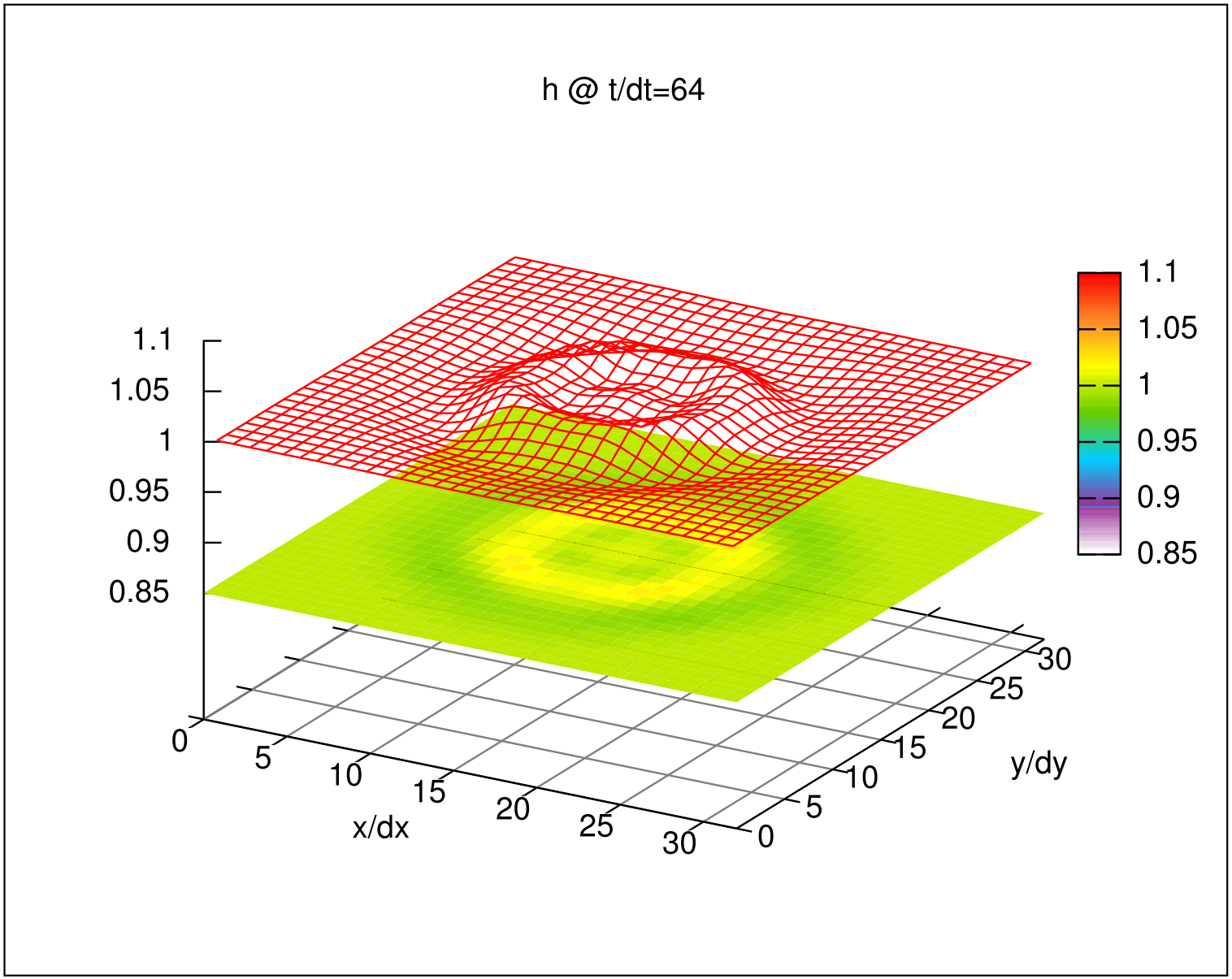

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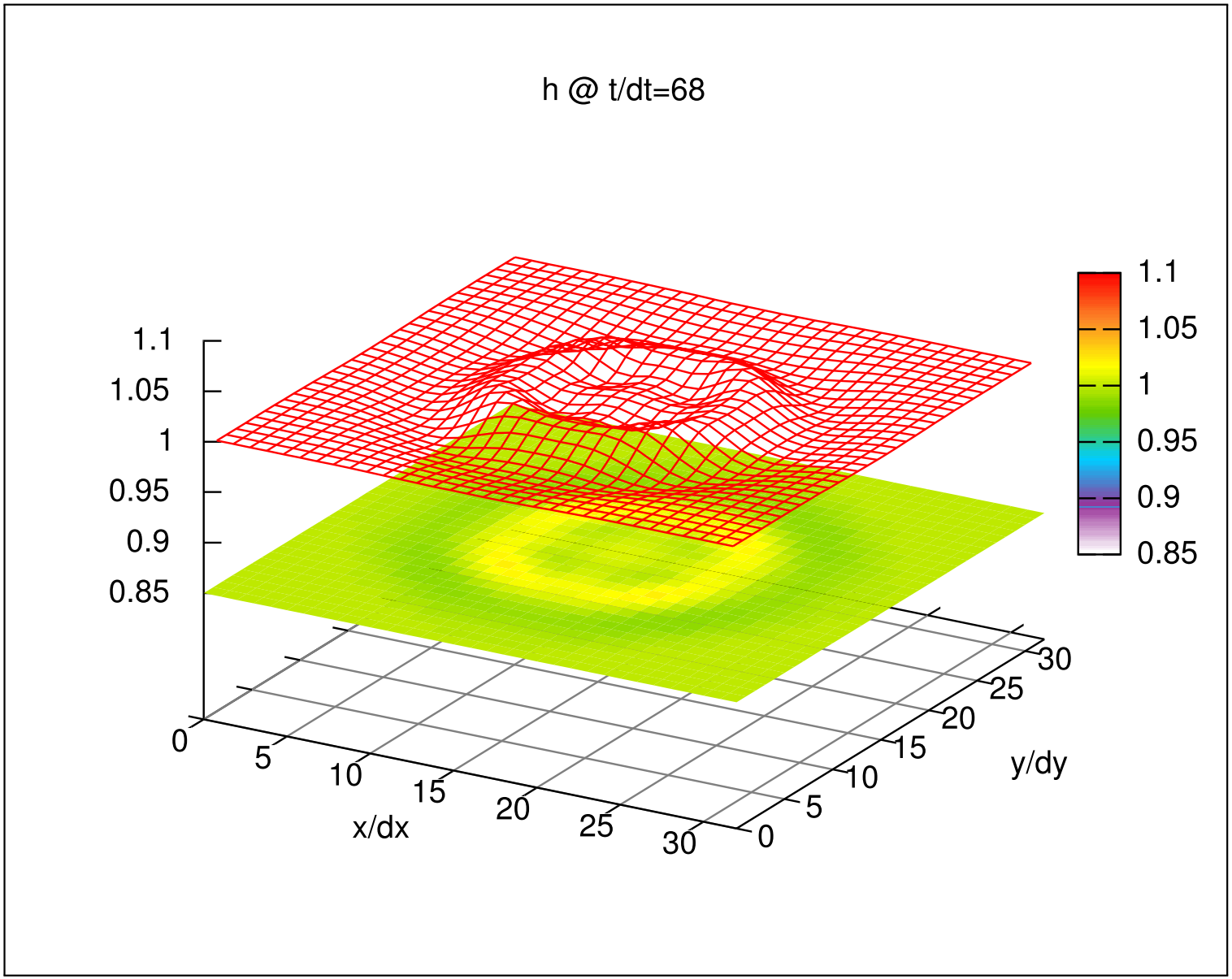

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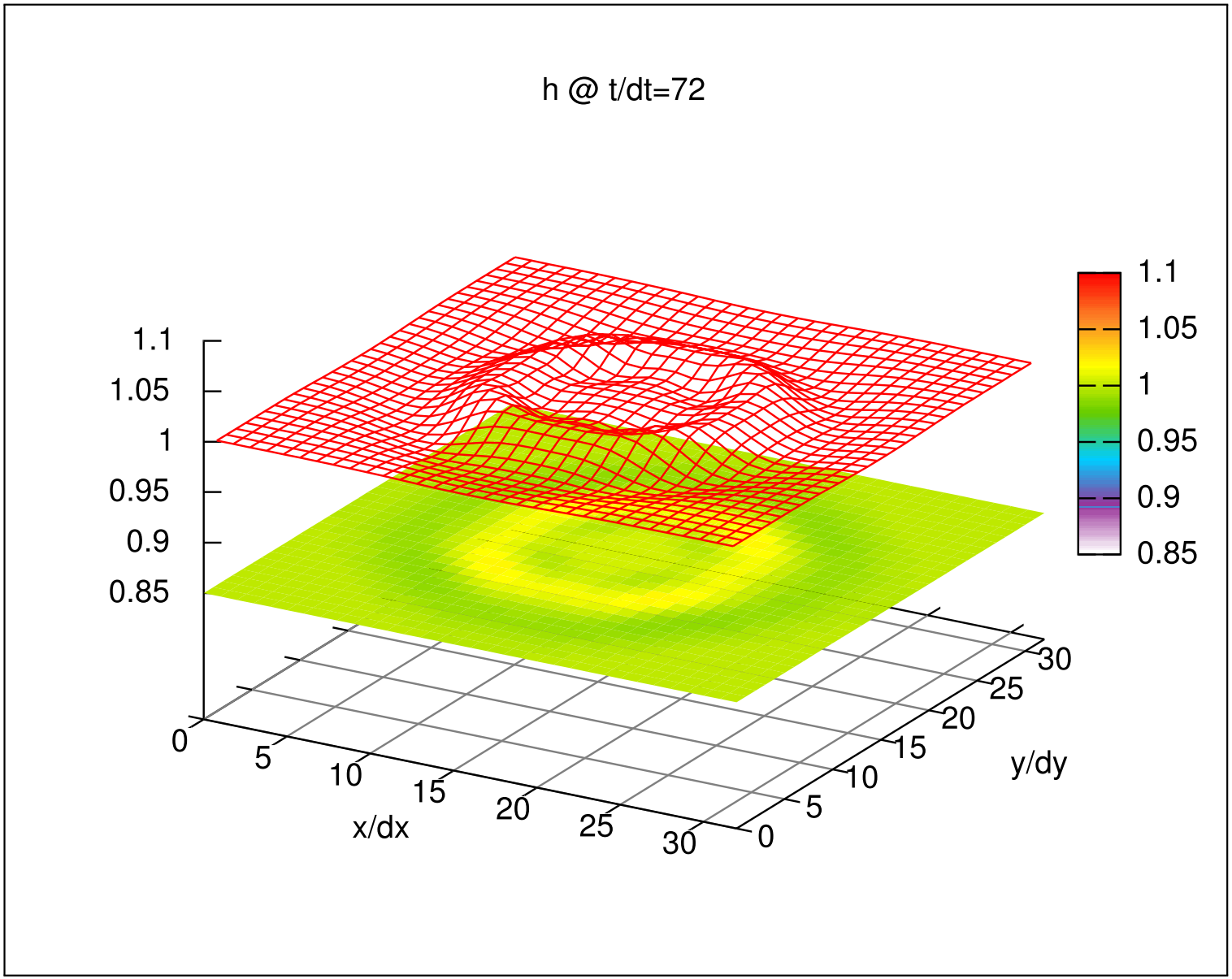

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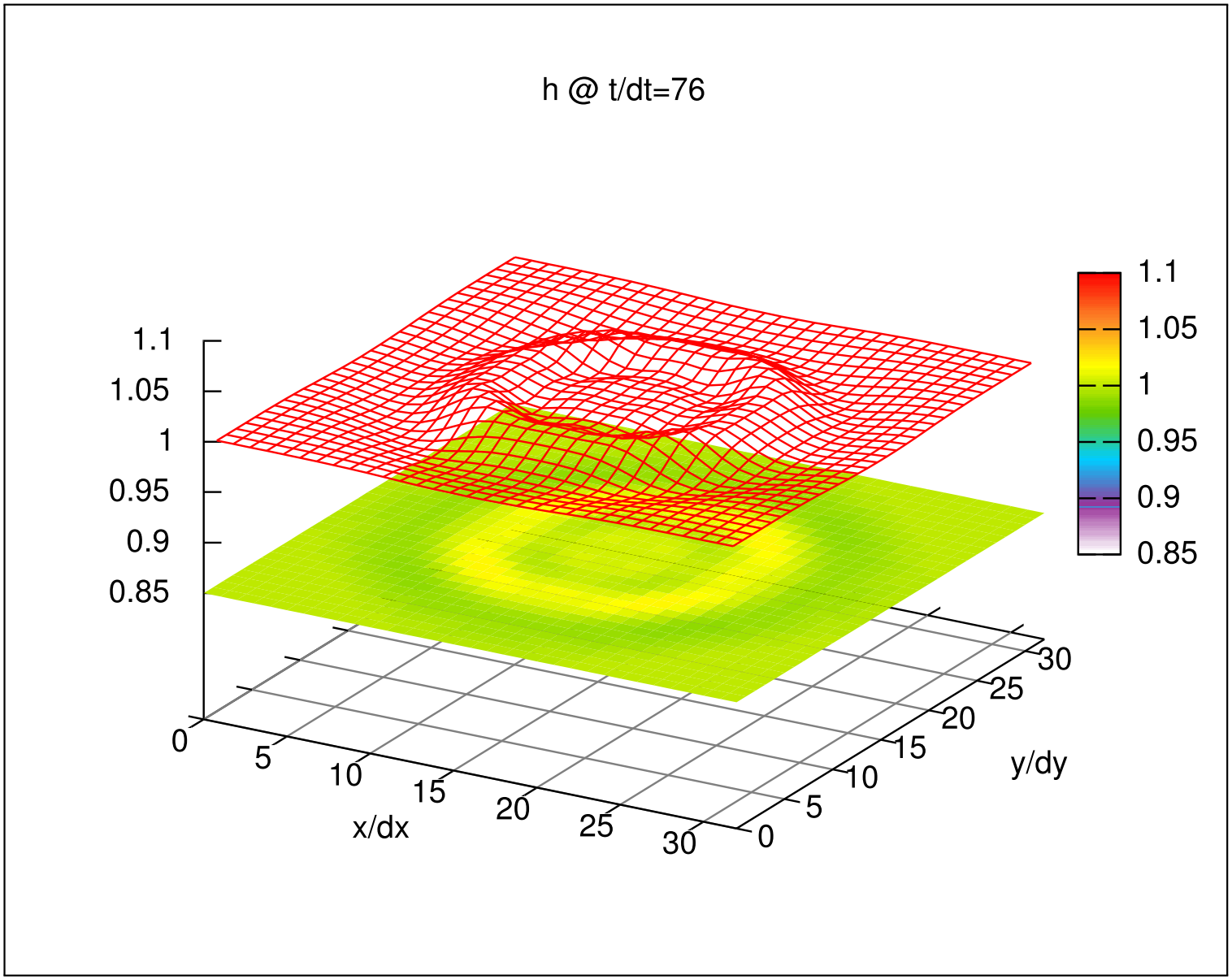

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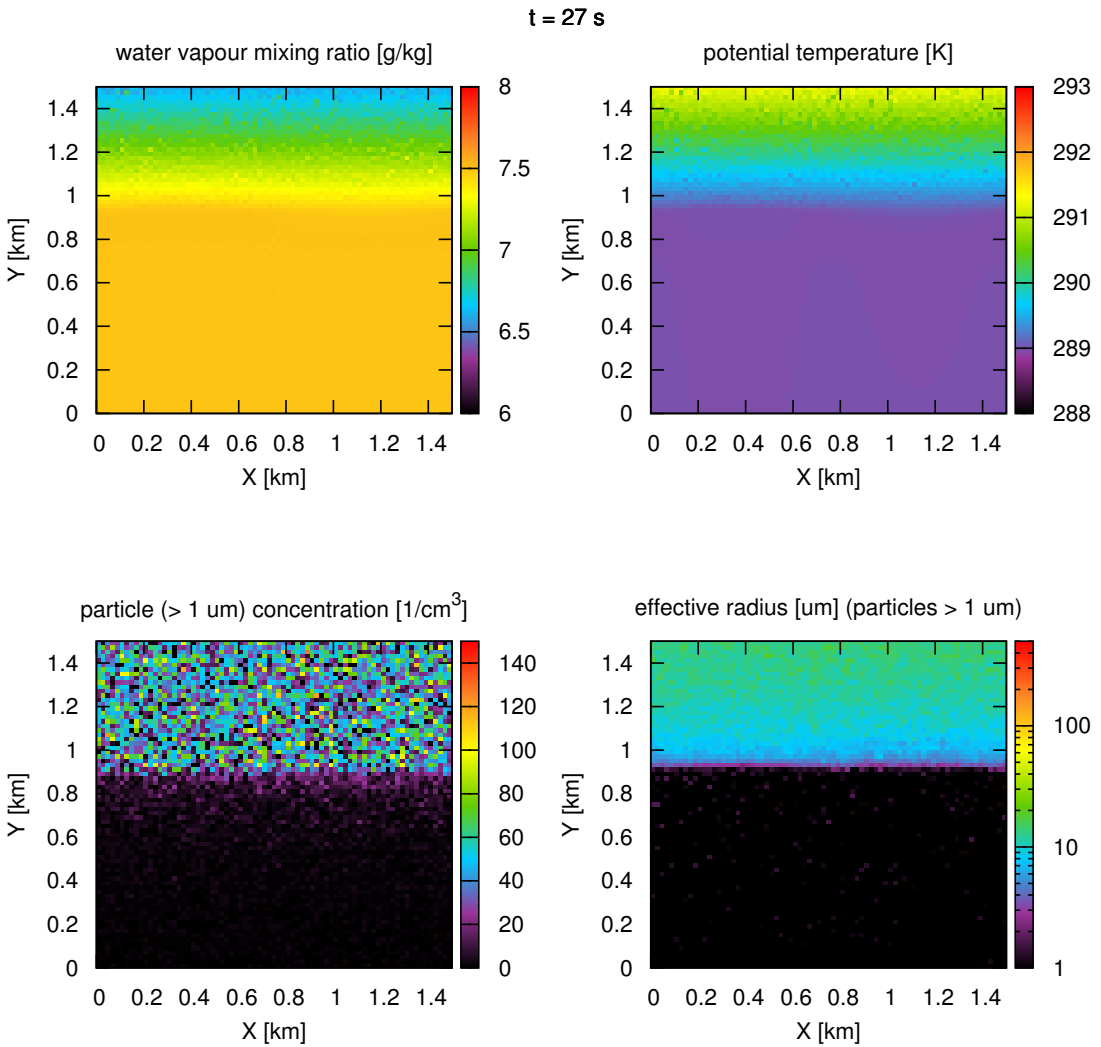

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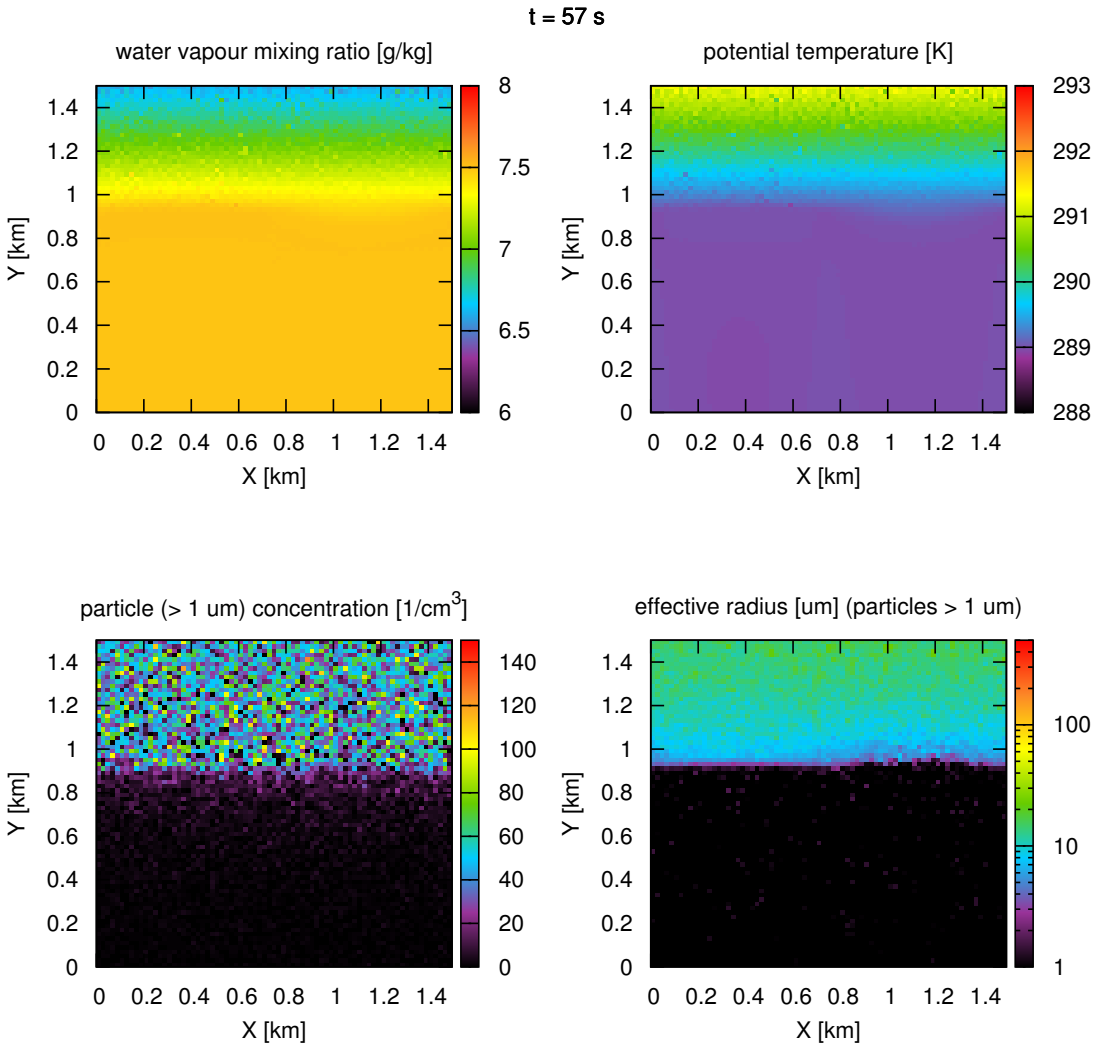

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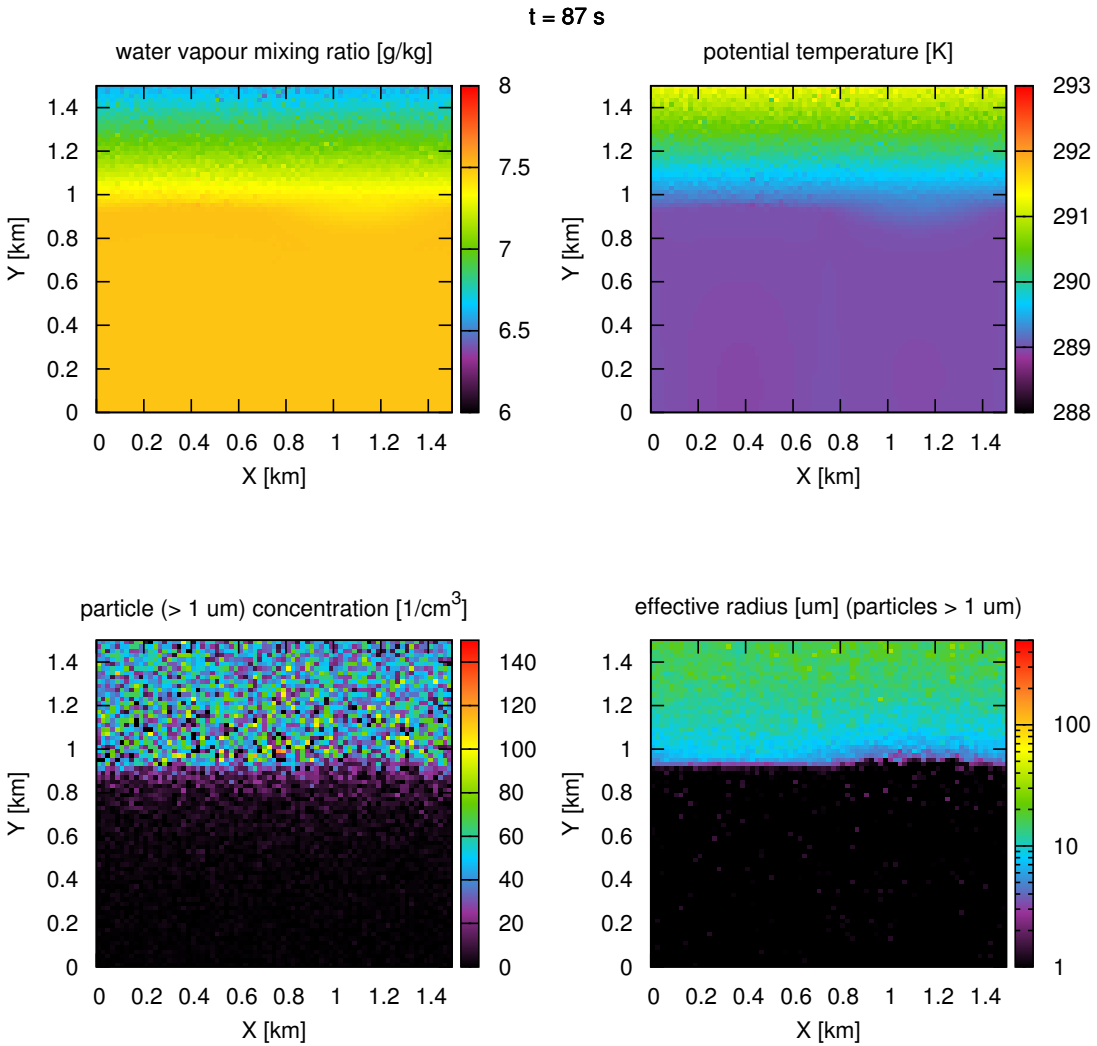

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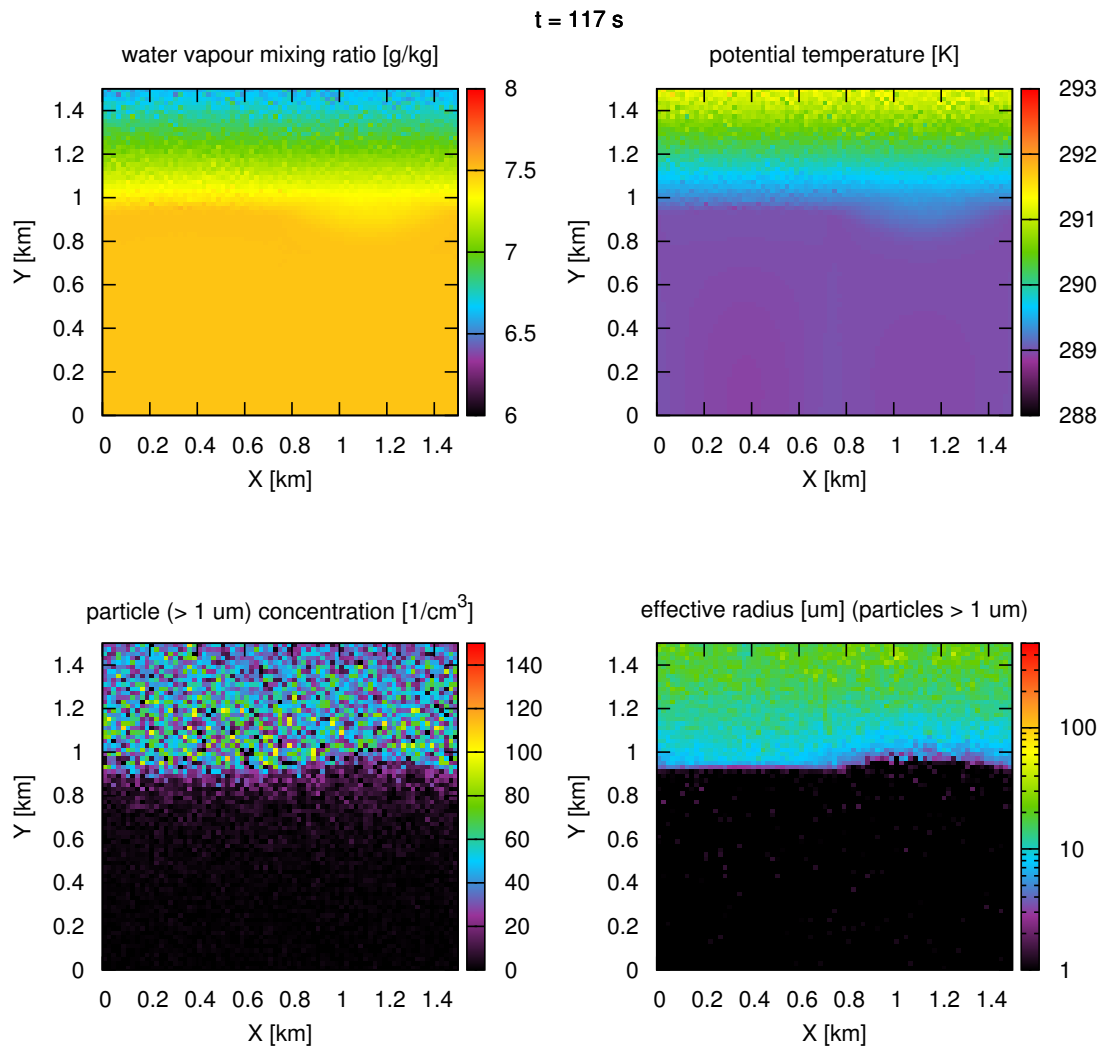

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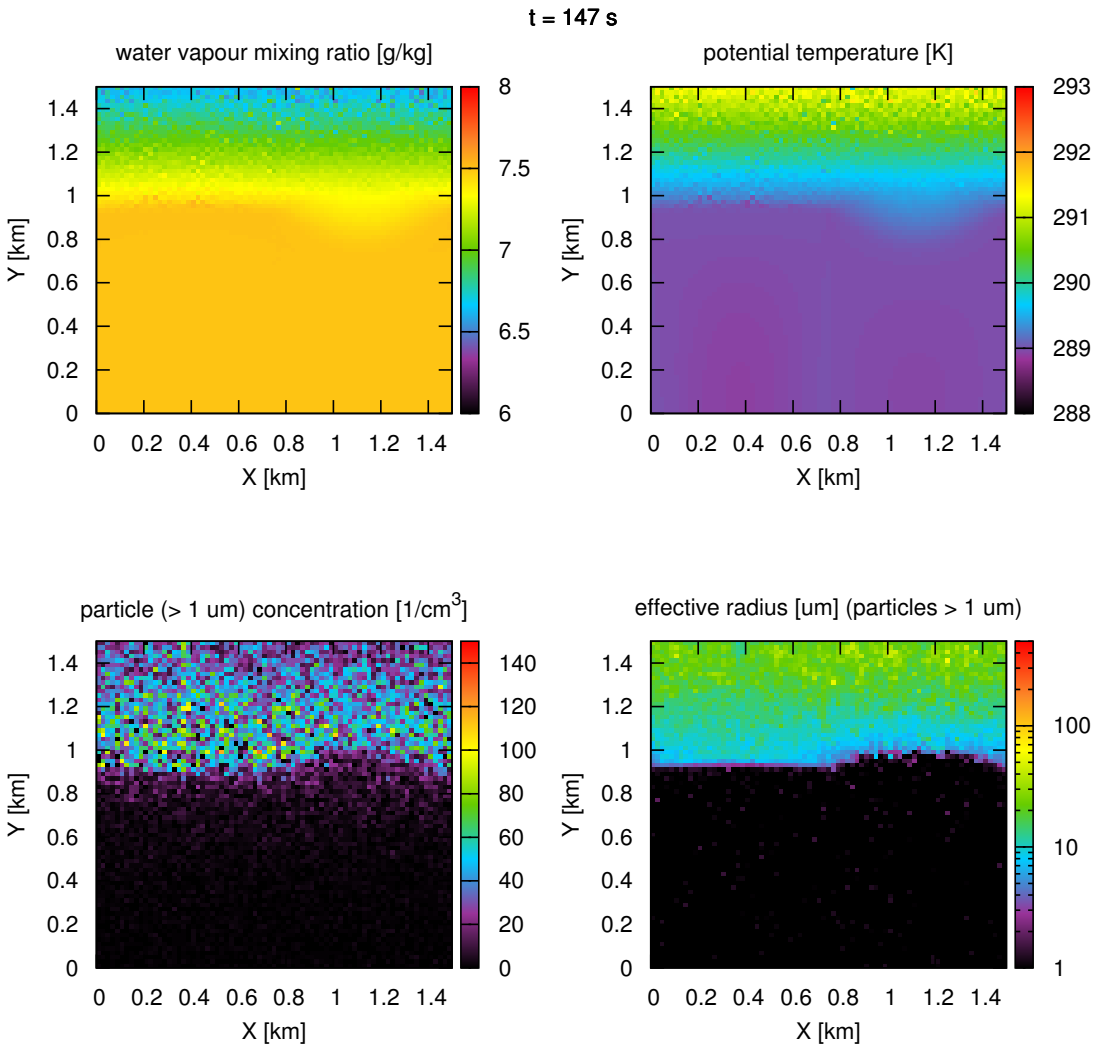

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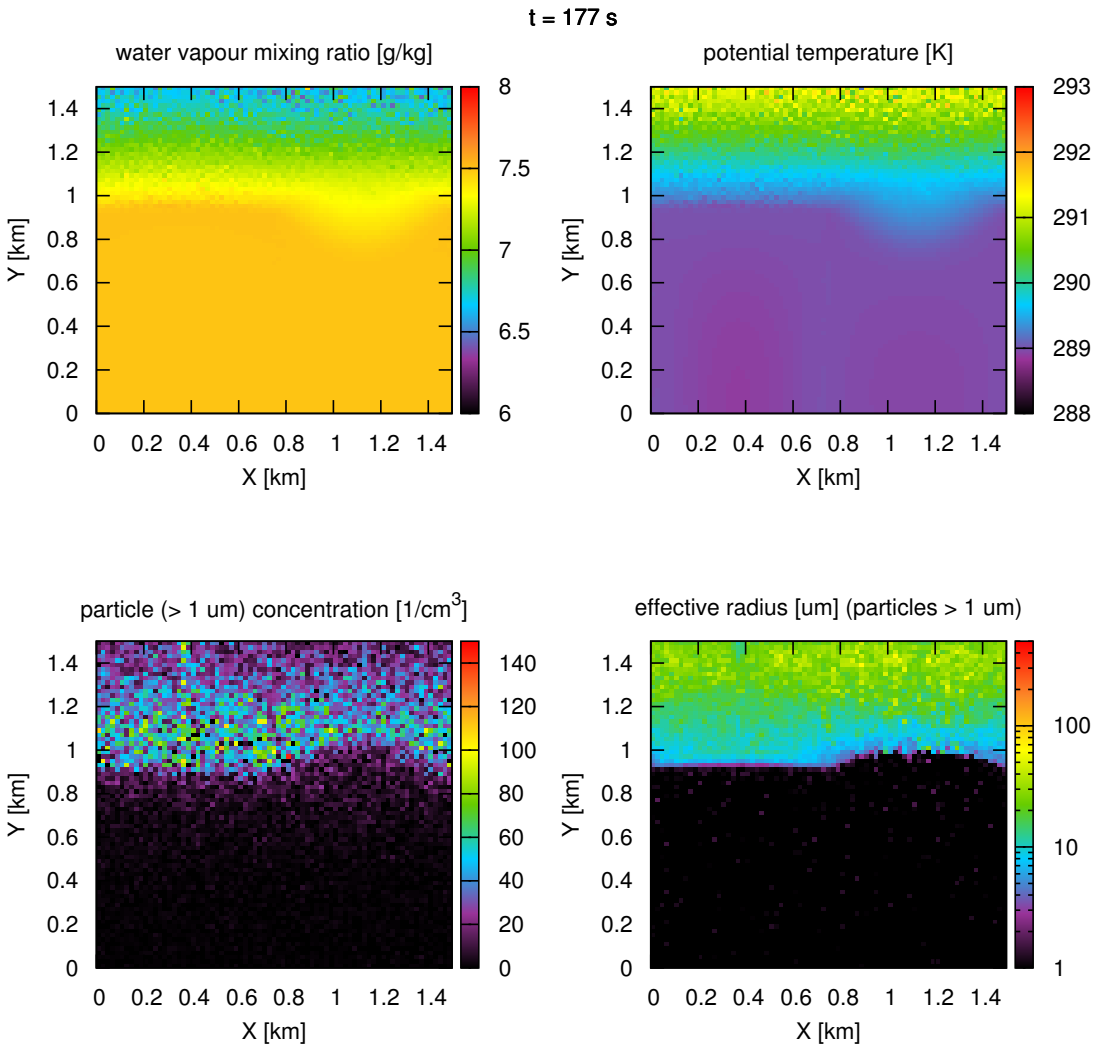

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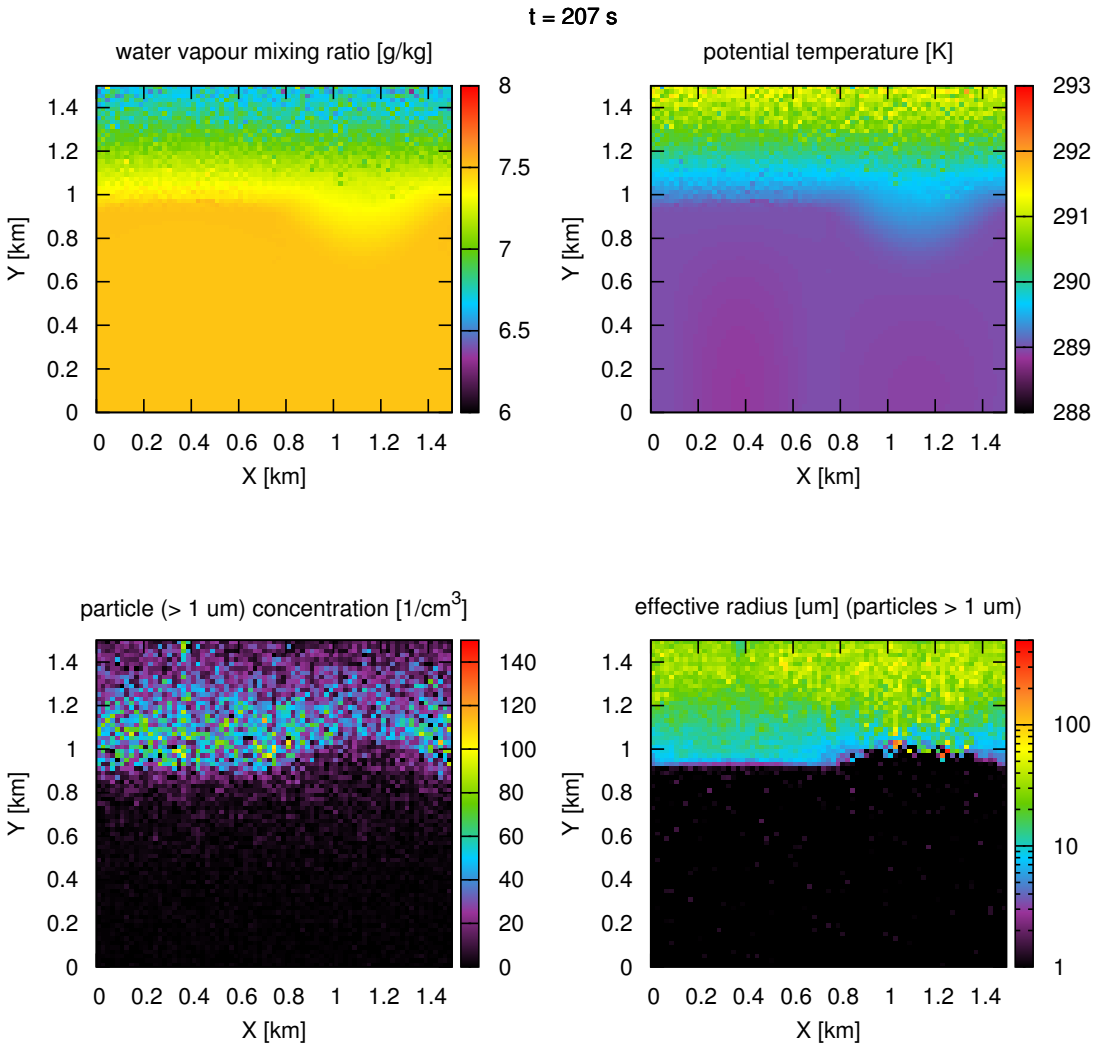

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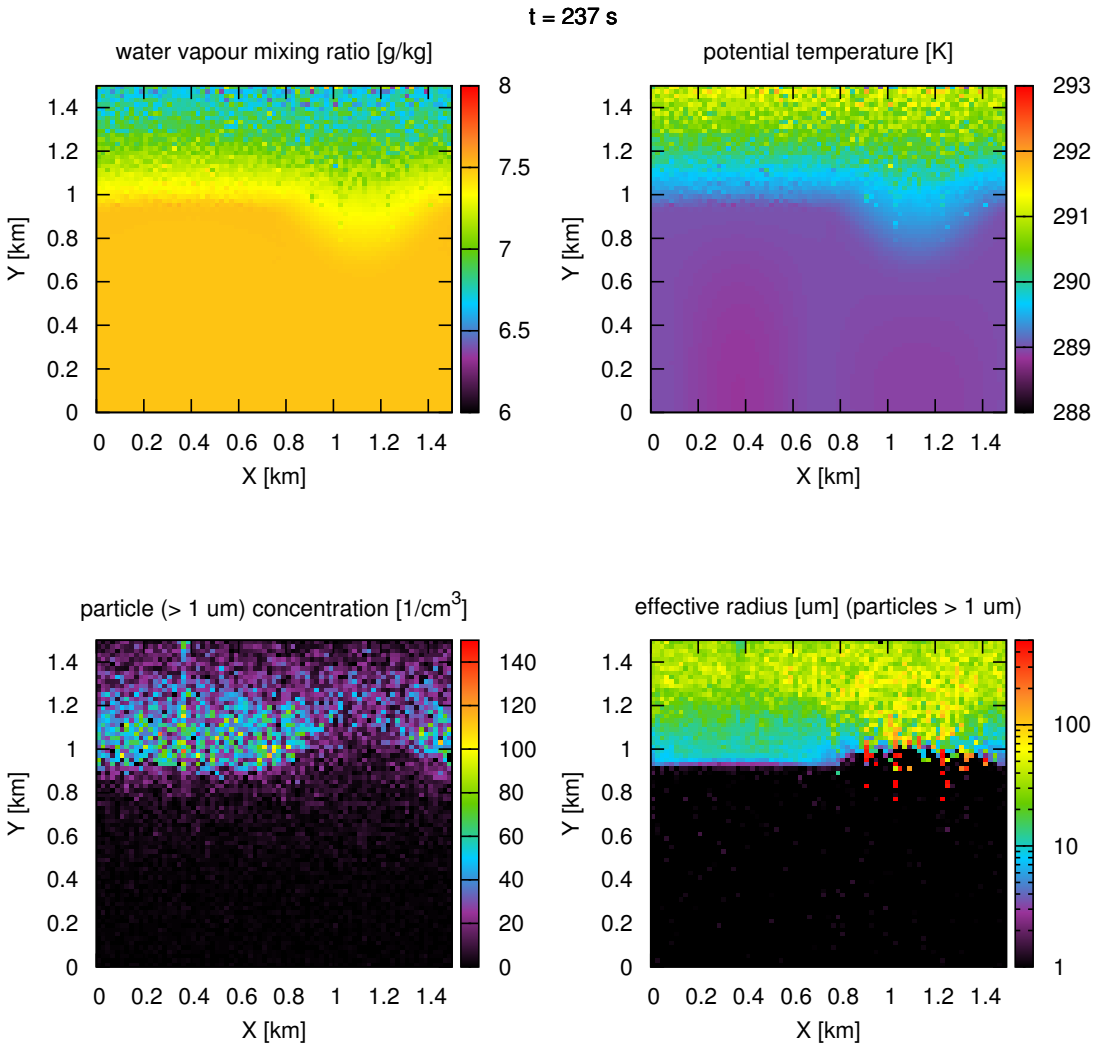

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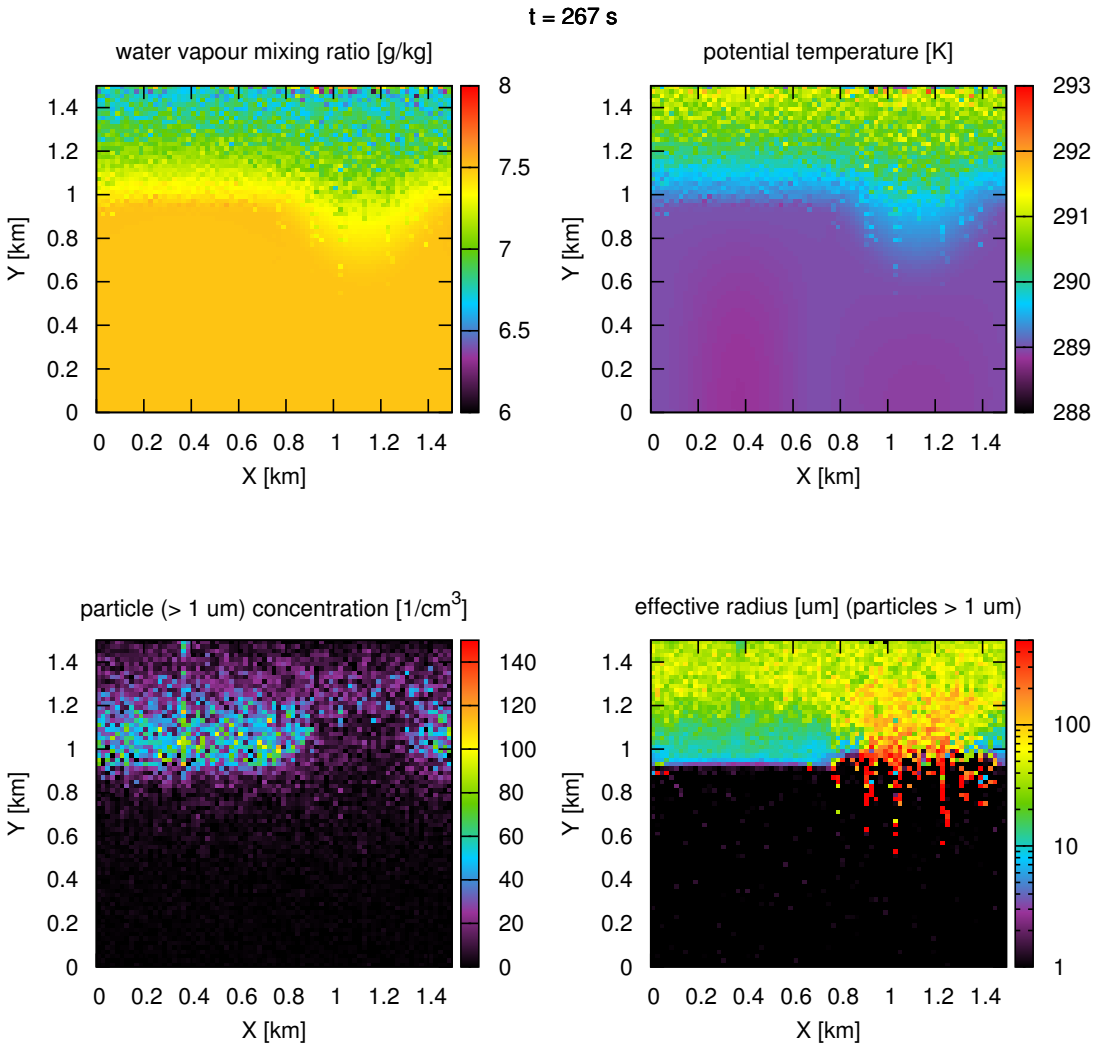

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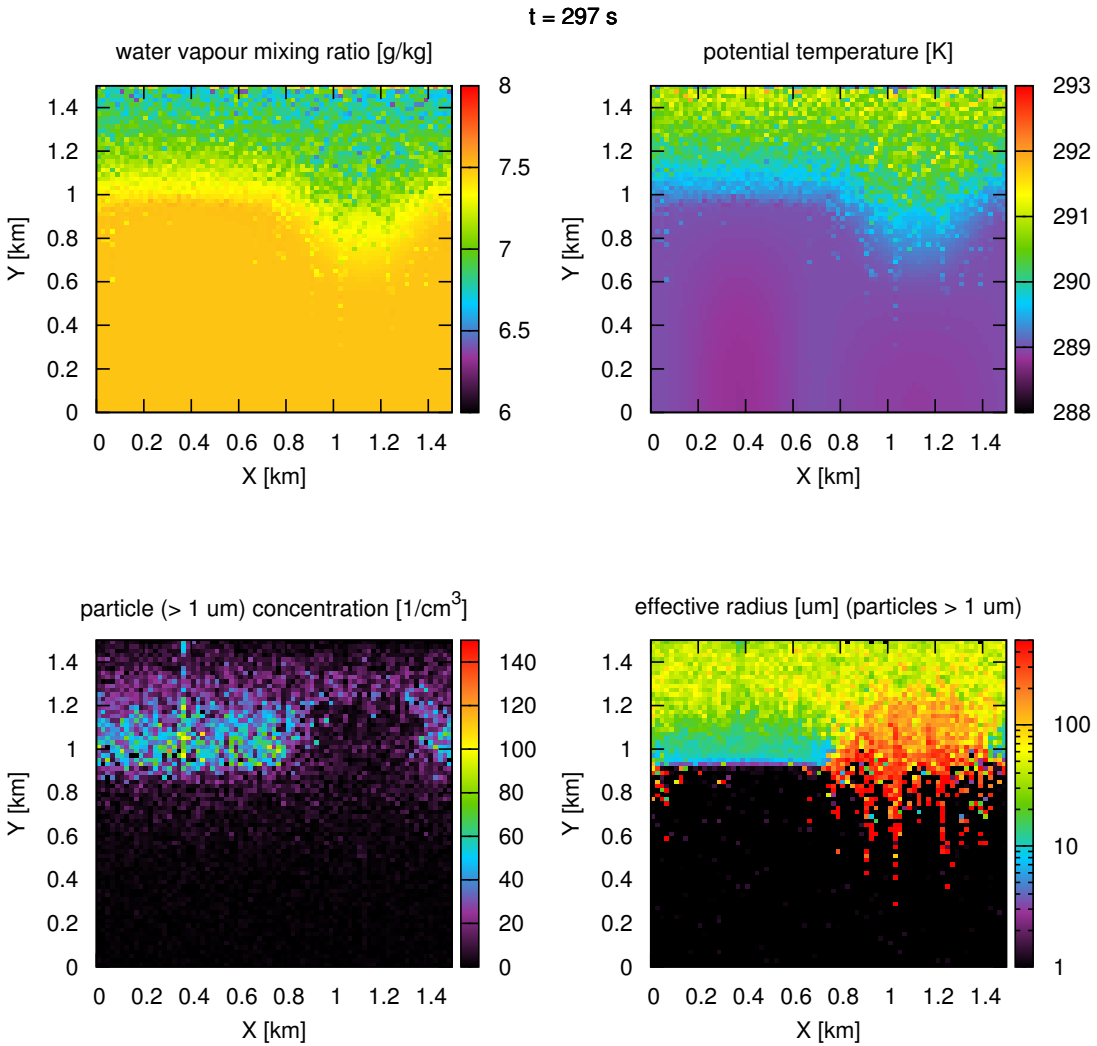

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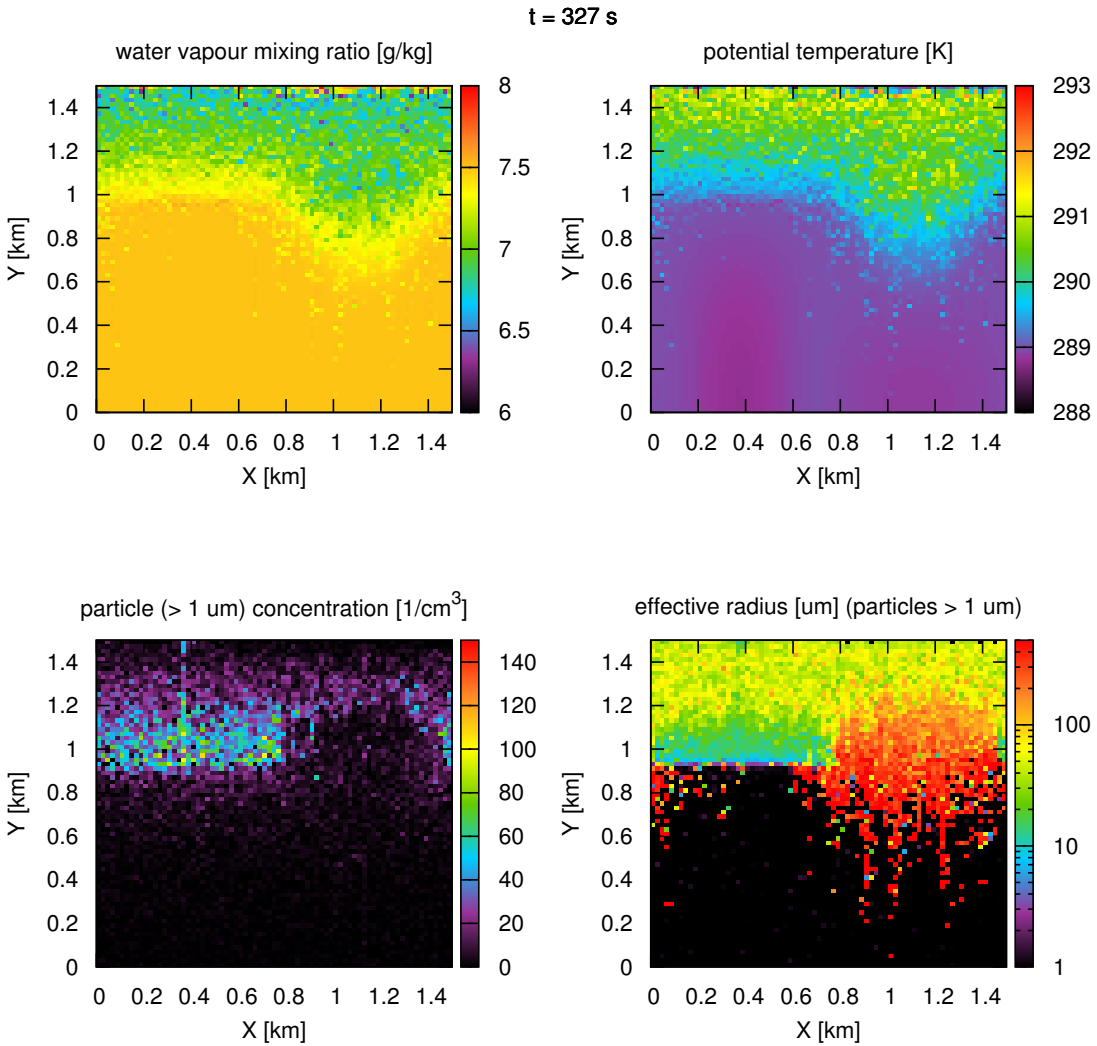

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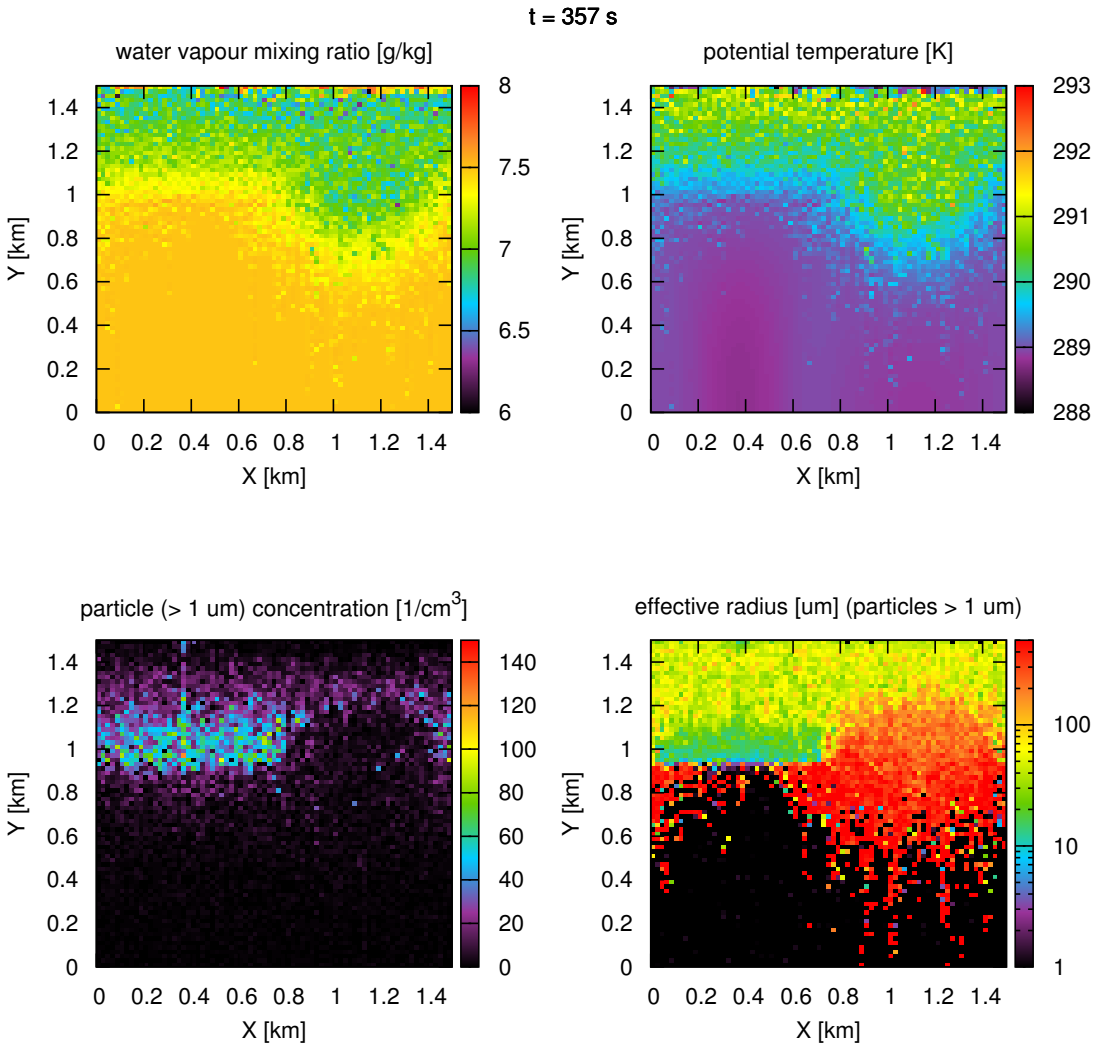

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- deps: libmpdata++, libcmphscs++, ...

icicLES OOP LES system for cloud-physics research

- deps: libmpdata++, libcmphscs++, ...
- news: Polish National Science Centre funds granted!
- plan: 3 years, ca. 3 full-time positions (50/50 sci/dev), co-op: Wojciech Grabowski, Piotr Smolarkiewicz

all GPL-licensed

a take-home message

C++11/Blitz++,
Python/NumPyPy,
and Fortran 2008

since very recently (2010s!)
offer similar and unprecedented possibilities
for matching the mathematical "blackboard abstractions"
in high-performance computing applications
using object-oriented programming

all are available as free & open-source solutions

cleverly used may significantly improve
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Thanks for your attention!

Contact: Sylwester Arabas / sarabas@igf.fuw.edu.pl

Paper: `http://arxiv.org/abs/1301.1334`

Co-authors:

- Dorota Jarecka & Anna Jaruga (Univ. Warsaw)
- Maciej Fijałkowski (PyPy team)

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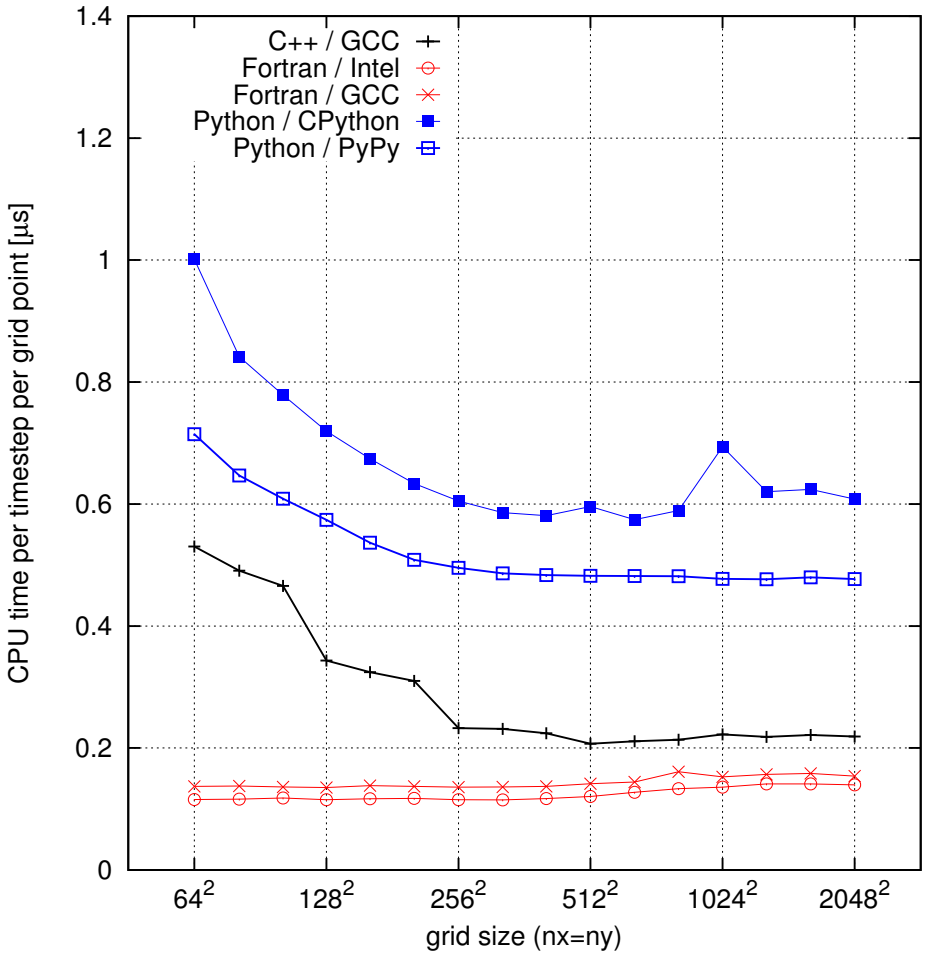
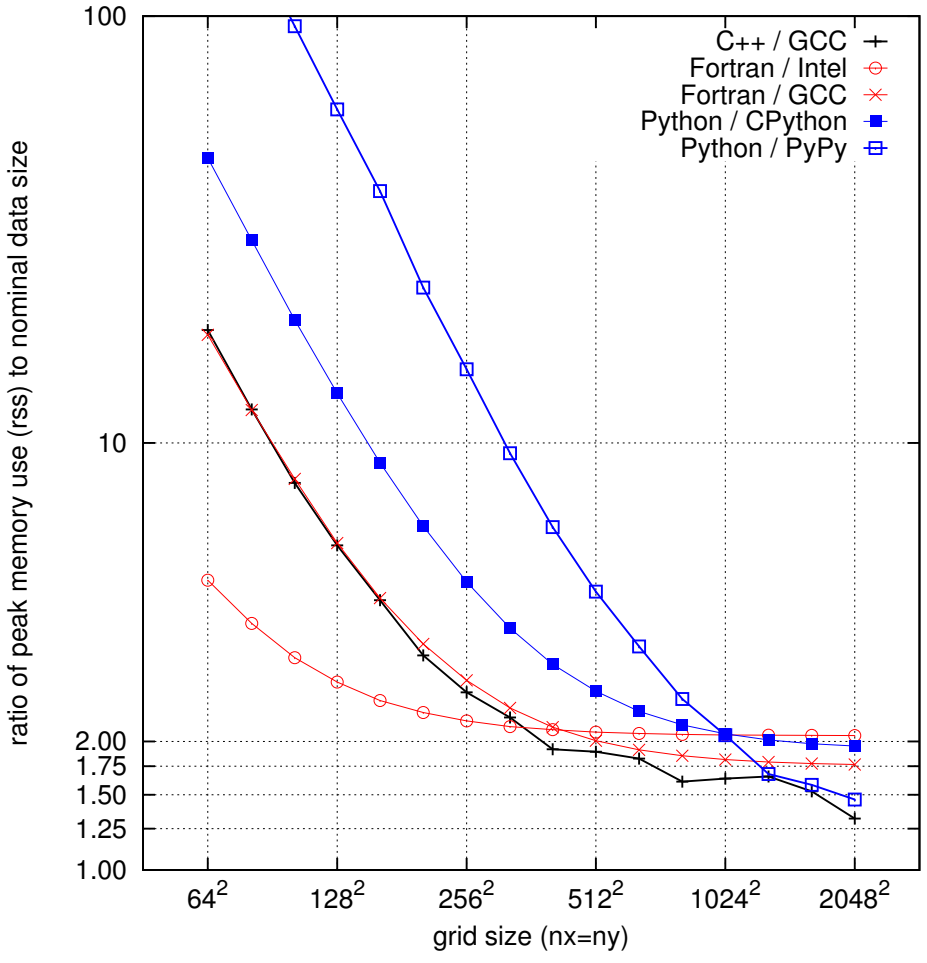
- UCAR/SEA for supporting my travel to US
- Piotr Smolarkiewicz for tutoring
- Hanna Pawłowska - head of our group @ Univ. Warsaw
- Polish National Science Centre for funding (2011/01/N/ST10/01483)
- Authors of free/libre open-source software used in the project

performance tests on yellowstone





g++/gfortran: -Ofast -march=native
ifort: -fast -axAVX

Thanks to Davide Del Vento!