Development and optimization of a coupled multi-GPU LBM-MHFEM solver for vapor transport in air

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Outline

Wind tunnel experiments

Joint work by Andrew C. Trautz[b] and Tissa Illangasekare[c]

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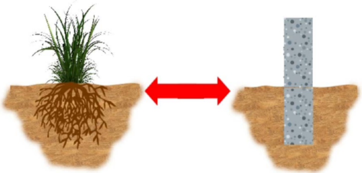
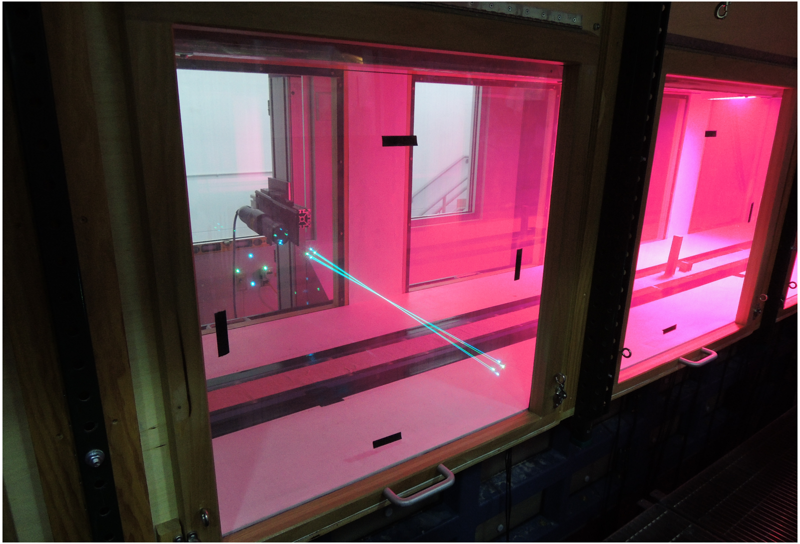
Experiments related to this talk:

- Climate-controlled, low-speed wind tunnel interfaced with a soil tank (CESEP, Colorado School of Mines, USA)
- Designed to study processes with mass flux across the land-atmospheric interface (e.g. water evaporation)
- Live vegetation approximated with limestone blocks

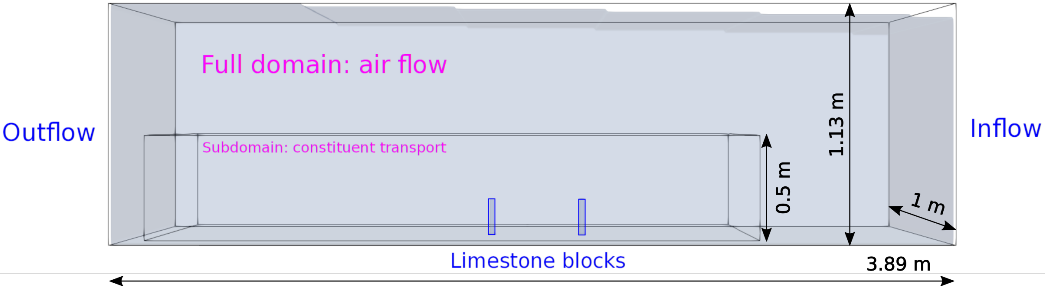


Wind tunnel experiments



Computational domain

Only part of the wind tunnel above soil surface; 2 identical blocks; different spacings.



Governing equations: air flow and vapor transport

NSE (air flow in $\Omega_1 \times (0, t_{\max})$):

$$\nabla \cdot \vec{v} = 0, \qquad (1a)$$

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = -\frac{1}{\rho} \nabla p + \nu \Delta \vec{v}, \qquad (1b)$$

ADE (vapor transport in $\Omega_2 \subset \Omega_1$):

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \vec{v} - D \nabla \phi) = 0, \qquad (2a)$$

Or in non-conservative form:

$$\frac{\partial \phi}{\partial t} + \vec{v} \cdot \nabla \phi - \nabla \cdot (D \nabla \phi) = 0. \qquad (2b)$$

- $\vec{v}$ **fluid velocity,**
- ρ fluid density,
- p fluid pressure,
- ν kinematic viscosity of the fluid,

- $\vec{v}$ **fluid velocity,**
- ϕ relative humidity,
- D diffusion coefficient.

Coupled LBM-MHFEM approach

- Equation (1) – lattice Boltzmann method (LBM)
  - D3Q27, Cumulant collision operator *(M. Geier et al., 2015)*
  - in-house code implementation *(R. Straka, R. Fučík, P. Eichler, J. Klinkovský et al.)*
  - implementation details later in this talk
- Equation (2) – mixed-hybrid finite element method (MHFEM)
  - *NumDwarf*: numerical scheme for a system of PDEs in a general-coefficient form
  - details in *R. Fučík, J. Klinkovský, J. Solovský, T. Oberhuber, J. Mikyška, Computer Physics Communications 238 (2019)*
- One-way coupling via the velocity field $\vec{v}$
  - Interpolation from the equidistant lattice to the MHFEM mesh

LBM-MHFEM: coupling details

Interpolation of the velocity $\vec{v}$:

- Trilinear or tricubic interpolation
- Evaluation at **cell side centers** (not cell centers) – to satisfy balancing requirements imposed by the MHFEM discretization

Transport equation:

- $\nabla \cdot \vec{v} = 0$ is not satisfied exactly by the LBM solver (weak compressibility)
- The interpolated velocity field is not locally conservative
- Numerical schemes for the **conservative and non-conservative variants are not equivalent**
- Solving the non-conservative rather than conservative transport equation gives more stable results

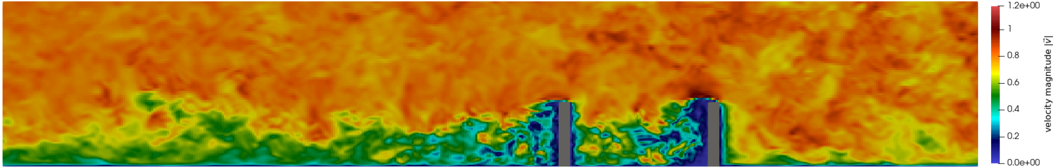
Time stepping:

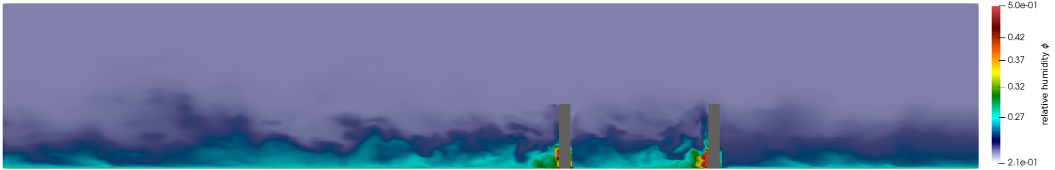
- MHFEM allows to use larger time steps than LBM
- **Adaptive time-stepping** strategy for MHFEM based on a CFL-like condition

Time-stepping algorithm

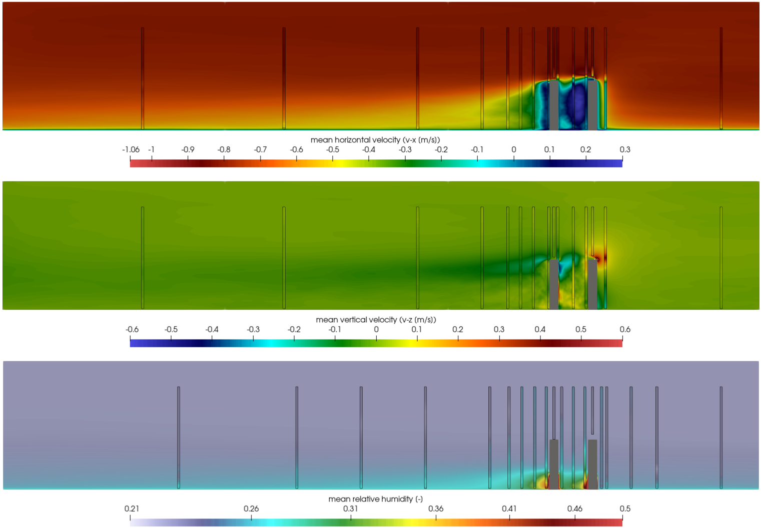
1. Set $t_L := 0$, $t_M := 0$, Δt and $t_{\max} = N_t \Delta t$
2. While $t_L < N_t \Delta t$, repeat these steps:
   1. Perform steps for one iteration of LBM (**details later**)
   2. Set $t_L := t_L + \Delta t$
   3. If $t_M < t_L$, perform these steps:
      1. Interpolate velocity from the lattice to the mesh.
      2. Compute $C = \max_E \{|\vec{v}_E| \Delta t / |E|\}$, where $E \in \mathcal{E}_h$ goes over all faces of the unstructured mesh
      3. Set the time step for MHFEM: $\Delta t_M := \Delta t \lfloor C_{\max}/C \rfloor$ if $C \le C_{\max}$, else $\Delta t_M := \Delta t / \lceil C/C_{\max} \rceil$
      4. Set the number of MHFEM iterations: $n_M := 1$ if $C \le C_{\max}$, else $n_M := \lceil C/C_{\max} \rceil$
      5. Perform n_M iterations of MHFEM with the time step Δt_M
      6. Set $t_M := t_M + n_M \Delta t_M$

Simulations – velocity and relative humidity profiles

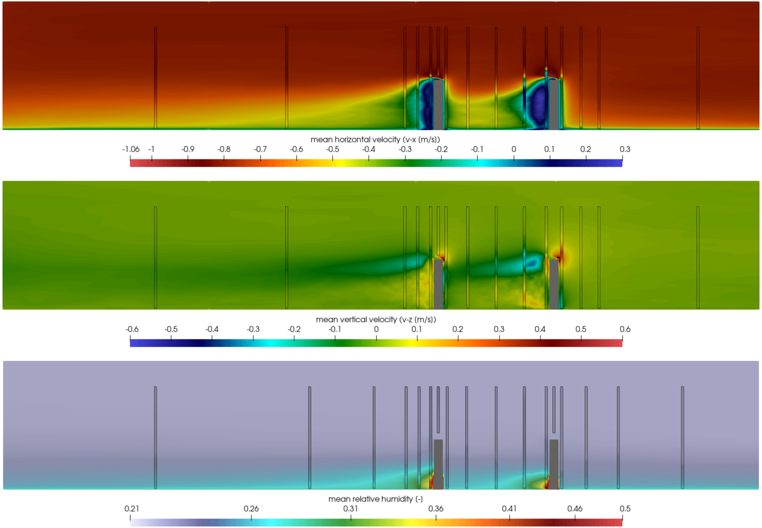




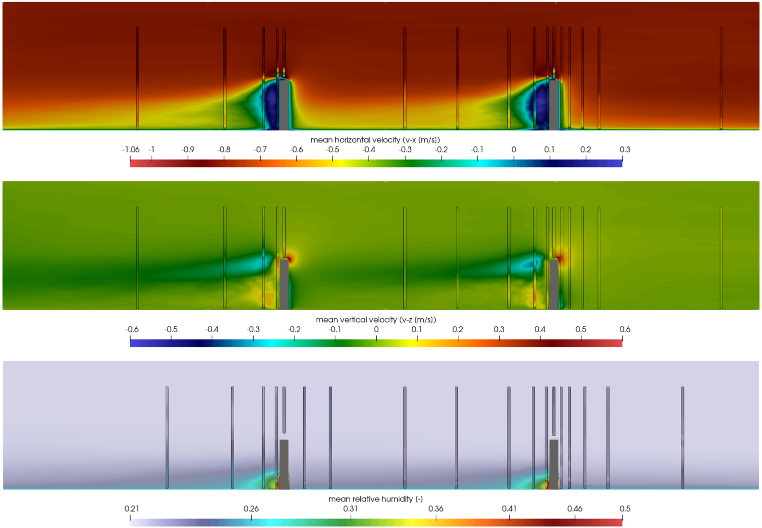
Qualitative comparison with experiment (EX-1: 15 cm)



Qualitative comparison with experiment (EX-2: 45 cm)

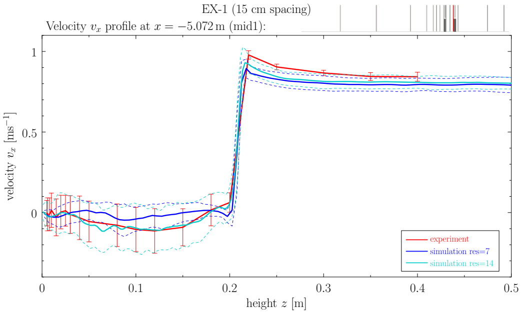


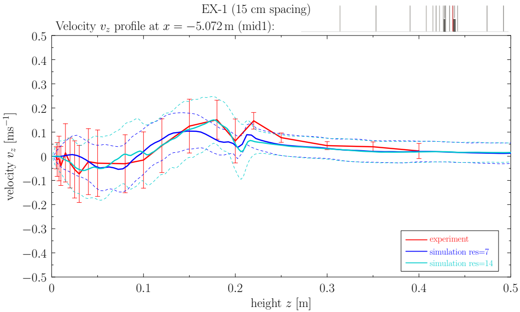
Qualitative comparison with experiment (EX-3: 105 cm)



Quantitative comparison with experiment (EX-1: 15 cm)

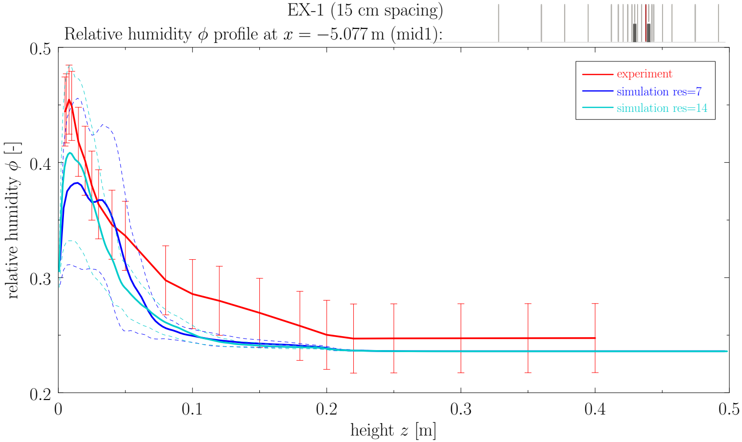
Horizontal and vertical velocity components:





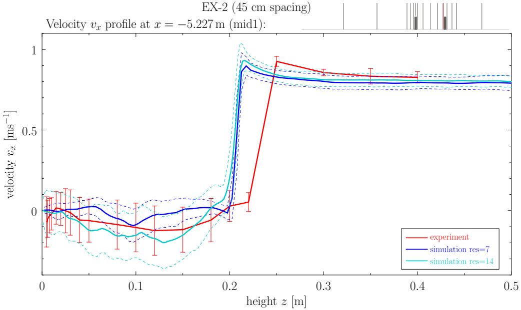
Quantitative comparison with experiment (EX-1: 15 cm)

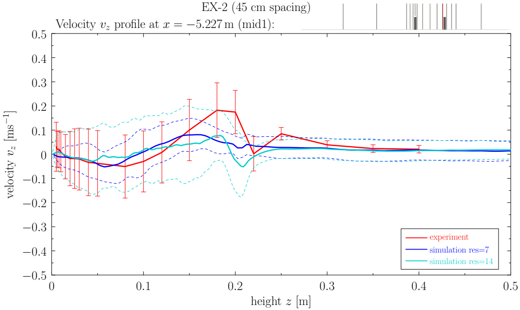
Relative humidity:



Quantitative comparison with experiment (EX-2: 45 cm)

Horizontal and vertical velocity components:





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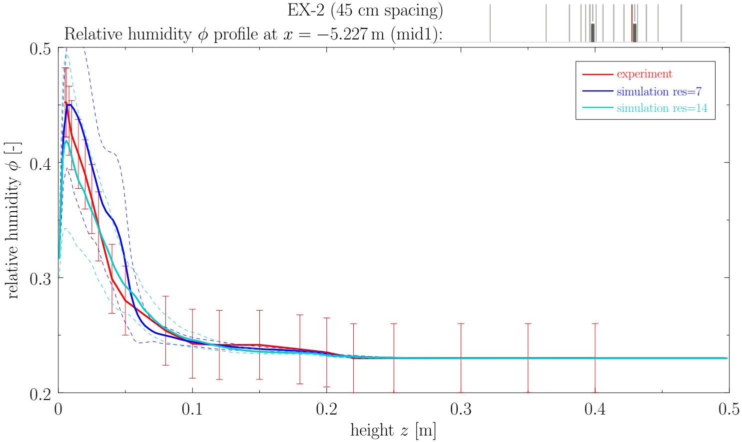

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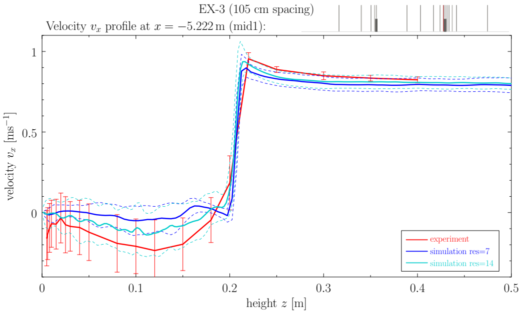

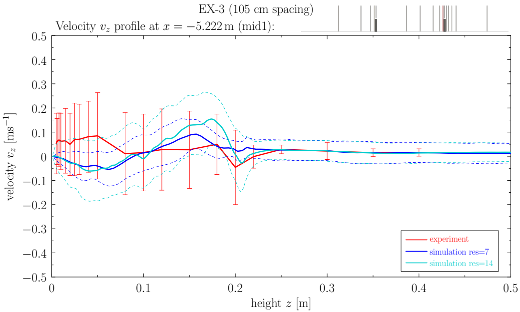

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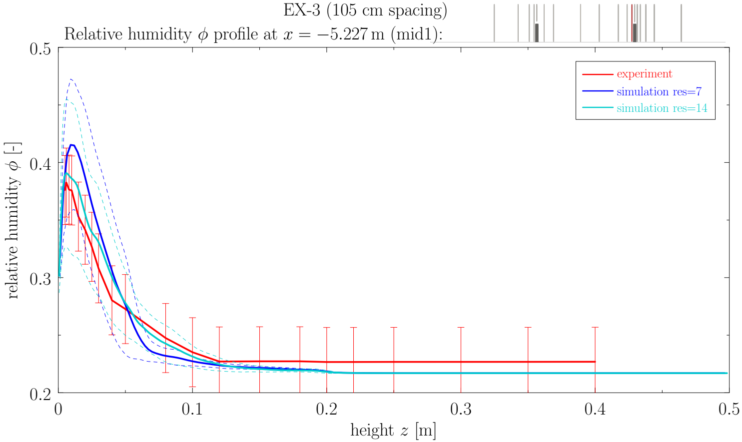


Implementation overview

Computation:

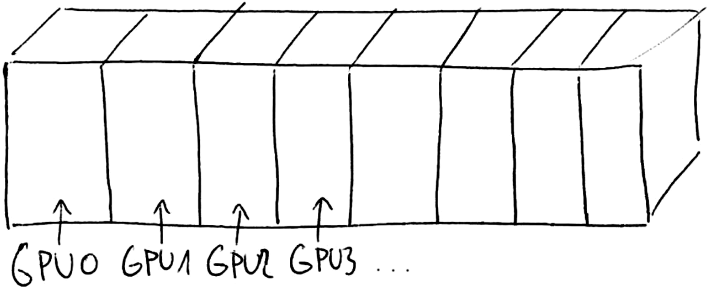
- All parts of the algorithm are computed on a GPU
- Multi-GPU implementation based on MPI

Custom code in C++ developed using:

- **Template Numerical Library**: `https://tnl-project.org/`
- **CUDA**: `https://docs.nvidia.com/cuda/`
- **Message Passing Interface**: `https://www.mpi-forum.org/`

Domain decomposition for LBM

- Computational domain = several independent subdomains + communication
- Computation: subdomains are processed on different GPUs
- Each MPI rank (process) manages its own GPU and subdomain
- Communication: 9 of 27 distribution functions need to be copied between adjacent subdomains
- For simplicity: only 1D distribution (our current implementation)

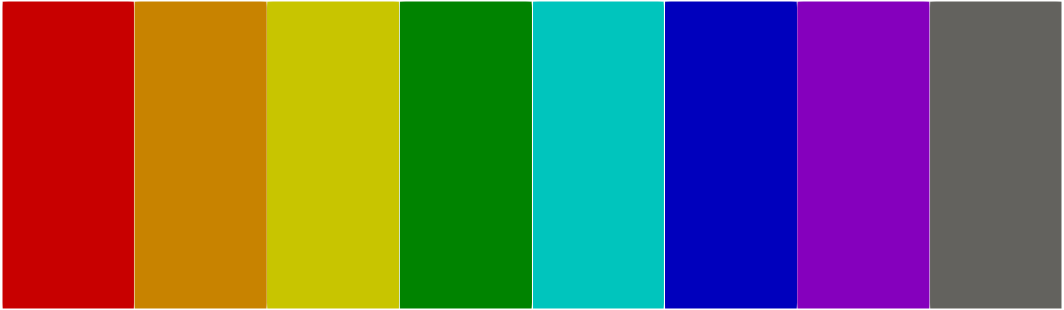


Implemented optimizations

- Domain decomposition with overlapped computation and communication (implementation based on CUDA streams)
- Avoiding buffers in communication (specific ordering of data in multidimensional arrays is necessary)
- Direct GPU-GPU copies via "CUDA-aware" MPI
- Streaming with the A-A pattern – reduced memory requirements
- **Balancing decomposition of the lattice and mesh**

Balancing decomposition of the lattice and mesh

Uniform lattice decomposition: 1/8 of nodes in each subdomain



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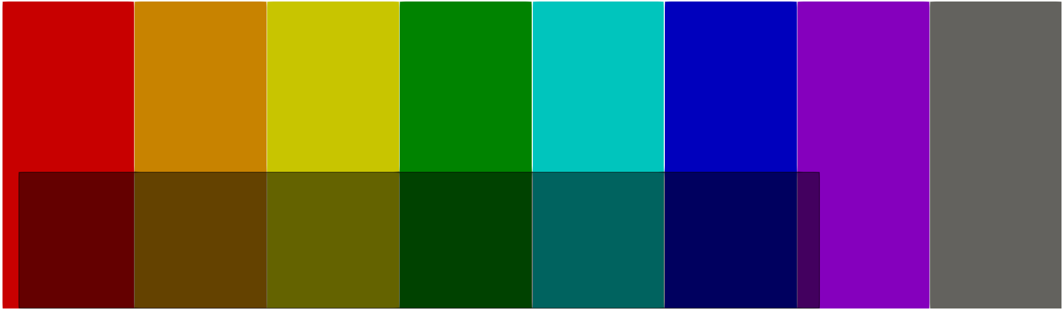
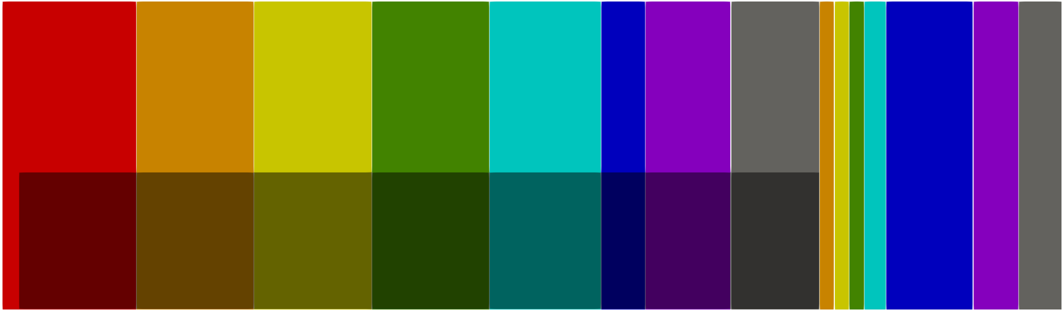


Unstructured mesh decomposition: non-uniform counts of mesh cells

12% 14% 14% 14% 24% 19% 3% 0%

Balancing decomposition of the lattice and mesh

Balanced lattice and mesh decomposition:



Approx. 1/8 of mesh cells **and** approx. 1/8 of lattice nodes per MPI rank.

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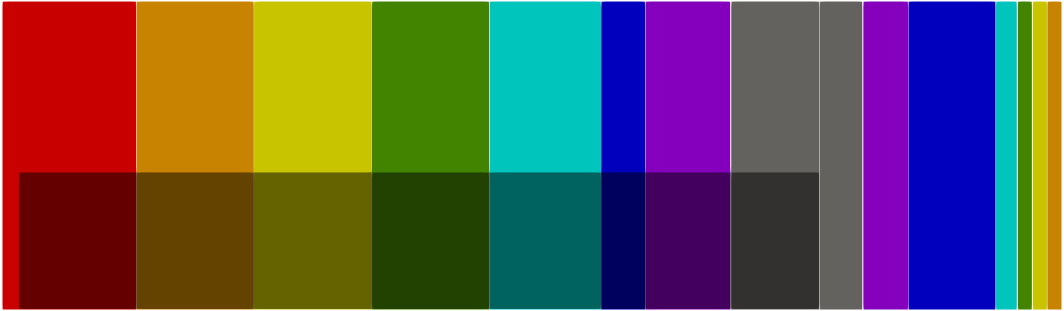

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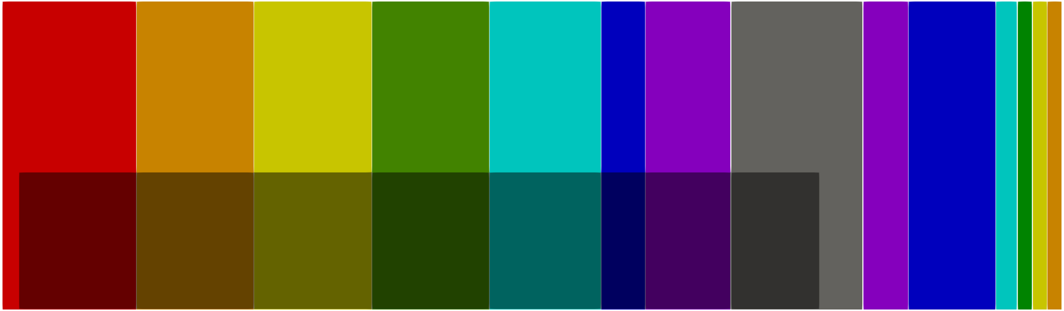

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Sketch of the decomposition algorithm

Approx. 500 lines of `C++` code:

1. Find the range $[x_1, x_2]$ where the lattice and mesh overlap
2. Define function $F(x) =$ [no. of mesh cells whose centroid is $\leq x$]
   (evaluated on lattice coordinates x_i and interpolated for $x \in \mathbb{R}$)
3. Define **objective function** $f : \mathbb{R}^{N_\text{ranks}} \mapsto \mathbb{R}$, where $N_\text{ranks} =$ [no. of MPI ranks]:
   - input variable $\vec{w}$, where $w_i \in \mathbb{R}$ stands for the width of i-th subdomain
   - imbalance on subinterval $[a, b]$ in the partitioning $= N_\text{ranks} \frac{F(b) - F(a)}{F(x_2) - F(x_1)} - 1$
   - $f(\vec{w}) = [\ell^2$ norm of mesh imbalances for partitioning $\vec{w}]$
4. Minimize f using the **gradient descent** method and the uniform partitioning as initial condition
5. Round the solution from $\mathbb{R}$ to the lattice coordinates (from `double` to `int`)
6. Try to increment/decrement each component of the solution and check if it improves the partitioning (iterative post-optimization in integer precision)
7. Decompose the remaining parts of the lattice which do not overlap with the mesh

Decomposition notes

- Amount of work optimized at the cost of increased communication
- Only 1D decomposition is currently implemented – not scalable
- Tested with up to 16 GPUs (Nvidia A-100) on 2 nodes (RCI cluster on FEE CTU):
  - 16×40 GiB = 640 GiB memory on the GPUs
  - Up to $3115 \times 800 \times 905 \approx 2.25 \times 10^9$ lattice nodes + approx. 48×10^6 mesh cells
  - Computational time: 52 hours (simulation of 100 s physical time)
- Not tested on more GPUs/nodes due to cluster limitations:
  - global allocation limit: only 20 GPUs per user job
  - only 2 nodes have usable inter-node GPU-GPU MPI communication

Performance results (RCI cluster on FEE CTU)

LBM-only performance (i.e., not coupled with MHFEM) – **weak scaling**

NVIDIA Tesla V100:

N_{nodes}	N_{GPUs}	GLUPS	Eff
1	1	2.5	1.00
1	4	10.4	1.05
2	8	19.3	0.97
4	16	39.4	0.99
8	32	50.1	0.63

NVIDIA Tesla A100:

N_{nodes}	N_{GPUs}	GLUPS	Eff
1	1	4.8	1.00
1	2	9.8	1.02
1	4	?.?	
1	8	?.?	

LBM-MHFEM performance – **strong scaling**

Weak scaling study is not possible due to different time steps in the MHFEM part.

N_{nodes}	N_{GPUs}	GLUPS	Eff
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Conclusion

- Validated model for vapor transport in air based on LBM and MHFEM
- Fully multi-GPU solver with good scalability on small number of GPUs

Future work:

- Development of the model (thermodynamics, coupling with porous media, etc.)
- Optimizations for scalability on more GPUs (e.g. multidimensional decomposition)

Thank you for your attention!

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- Czech Science Foundation (project 21-09093S)
- Ministry of Education, Youth, and Sports of the Czech Republic (Inter-Excellence grant LTAUSA19021, OP RDE grant CZ.02.1.01/0.0/0.0/16_019/0000765)
- Grant Agency of the Czech Technical University in Prague (project SGS20/184/OHK4/3T/14)

Related papers:

- J. Klinkovský, A. C. Trautz, R. Fučík, T. H. Illangasekare: Lattice Boltzmann Method–Based Efficient GPU Simulator for Vapor Transport in the Boundary Layer Over a Moist Soil: Development and Experimental Validation, in preparation
- R. Fučík, J. Klinkovský, J. Solovský, T. Oberhuber, J. Mikyška: Multidimensional mixed-hybrid finite element method for compositional two-phase flow in heterogeneous porous media and its parallel implementation on GPU, Computer Physics Communications, 2019