

Accurate curved Dirichlet boundaries for fluid flow simulations on the lattice Boltzmann uniform Cartesian grid

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Outline



- 1 Introduction
- 2 The lattice Boltzmann equation
- 3 Boundary closure and accuracy
- 4 Classification
- 5 Stability
- 6 Results
- 7 The End

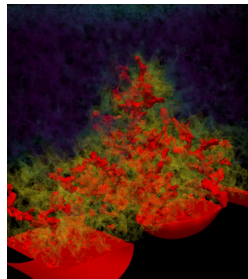
Lid driven cavity with Palabos on GPUs

💡 Lattice Boltzmann method → accurate complex boundaries with a **uniform Cartesian mesh**.

▶ What can we do with accurate directional boundary conditions on uniform grids?

⇒ High-performance high-fidelity multi-GPU simulations on uniform Cartesian grids!

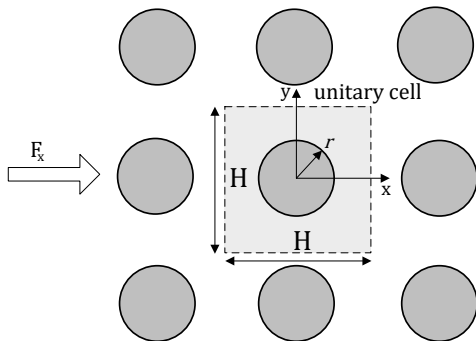
Example: porous media simulations with fully resolved geometries using Palabos (Latt et al., 2021)



<https://palabos.unige.ch/class/summer-school/>

Academic example for accuracy benchmarking

We perform a test to calculate the accuracy of the permeability for a flow around an array of cylinders.



The (forceless) lattice Boltzmann equation

BGK-LBE

$$f_i(\mathbf{x} + \mathbf{c}_i, t + 1) = \overbrace{f_i(\mathbf{x}, t)}^{\hat{f}_i(\mathbf{x}, t)} - \underbrace{\frac{n_i}{\tau}}_{\hat{n}_i}$$

$$n_i = f_i - e_i$$

TRT-LBE

$$f_i^\pm(\mathbf{x} + \mathbf{c}_i, t + 1) = \overbrace{f_i^\pm(\mathbf{x}, t)}^{\hat{f}_i^\pm(\mathbf{x}, t)} - \underbrace{\frac{n_i^\pm}{\tau^\pm}}_{\hat{n}_i^\pm}$$

$$\Lambda^\pm = \tau^\pm - 1/2, \quad \Lambda = \Lambda^+ \Lambda^-$$

collide: $f_i(\mathbf{x}, t) \rightarrow \hat{f}_i(\mathbf{x}, t)$

stream: $\hat{f}_i(\mathbf{x}, t) \rightarrow f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t)$

e_i = polynomial expansion of Maxwell-Boltzmann distribution

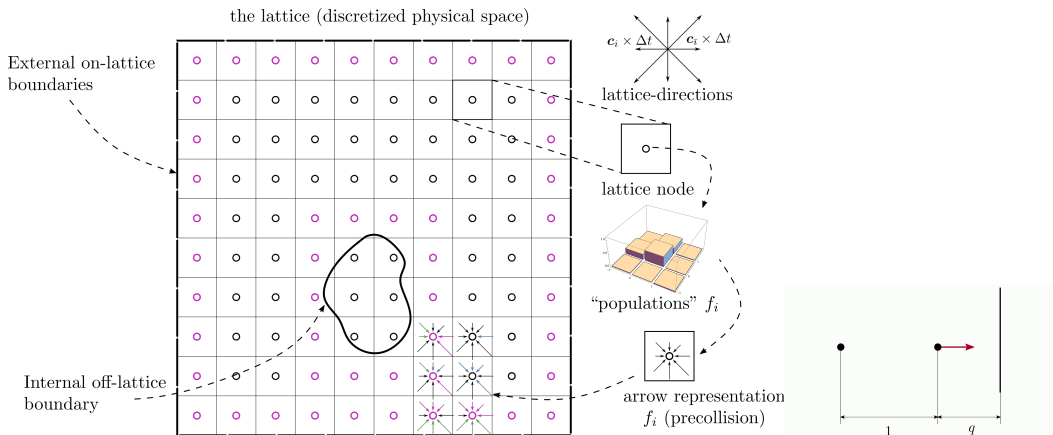
$e_{i,1}$ = linear equilibrium (truncation at the first order)

if D2Q9 $\rightarrow i \in \{0, \dots, 8\}$

The Lattice

$$f_i(\mathbf{x} + \mathbf{c}_i, t + 1) = \overbrace{f_i(\mathbf{x}, t)}^{\hat{f}_i(\mathbf{x}, t)} + \hat{n}_i$$

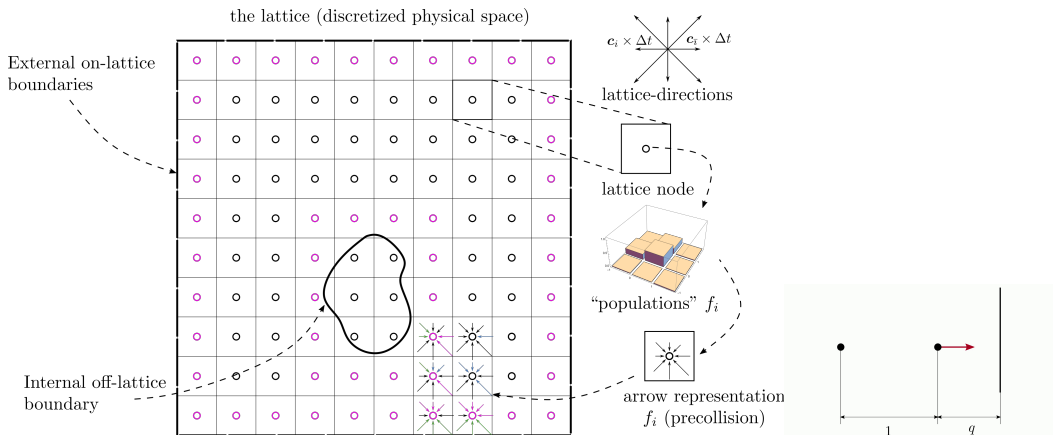
△ the difference between populations have been exaggerated to easy the recognition



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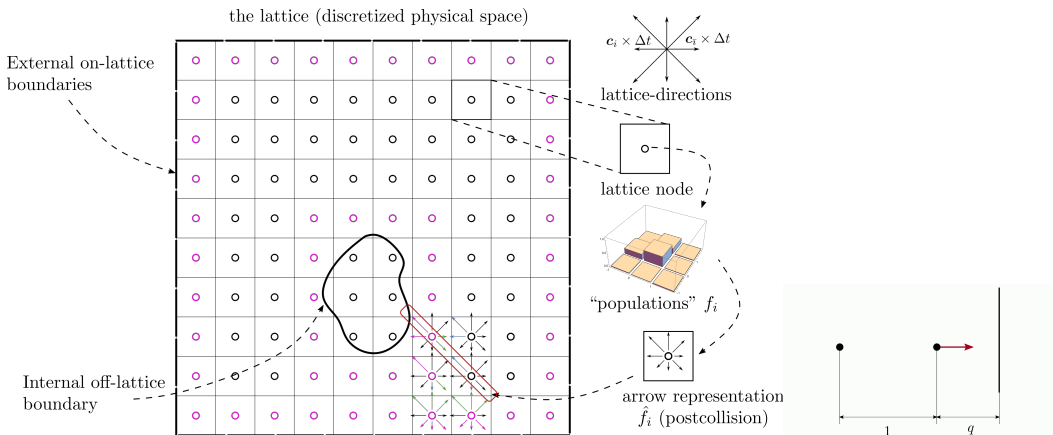
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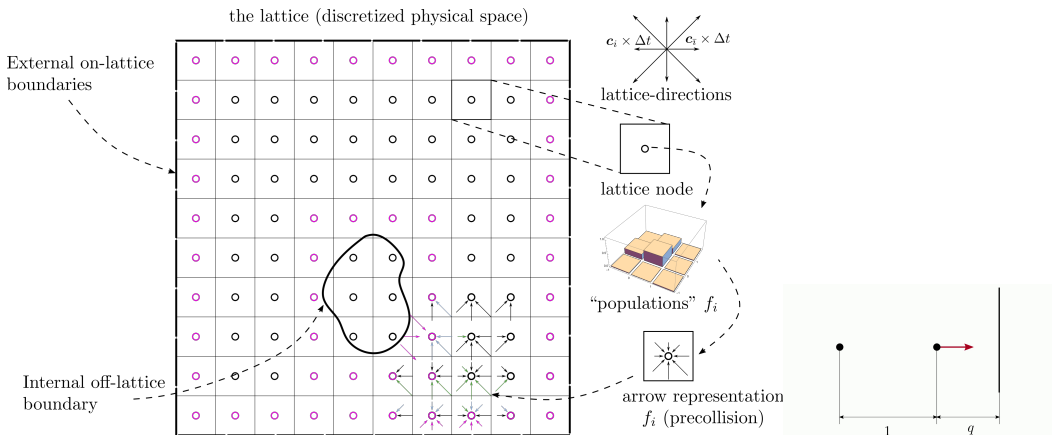
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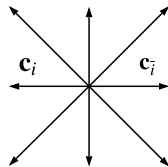
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Moments of the distribution function, solvability conditions

Macroscopic fields (without momentum and mass sources):

$$\rho = f_0^+ + 2 \sum_{i=1}^{Q_m/2} f_i^+, \quad P = c_l^2 \rho, \quad u_\alpha = 2 \sum_{i=1}^{Q_m/2} f_i^- c_{i,\alpha}$$



Solvability conditions:

$$\hat{h}_0^+ + 2 \sum_{i=1}^{Q_m/2} \hat{h}_i^+ = 0, \quad 2 \sum_{i=1}^{Q_m/2} \hat{h}_i^- c_{i,\alpha} = 0.$$

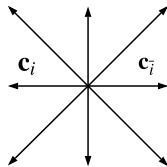
(Quasi-incompressible) equilibrium

$$e_i = e_i^+ + e_i^-$$

$$e_i^+ = w_i \rho + w_i \rho_0 l_{\text{Ma}^2} \underbrace{\frac{u_{\alpha_1} u_{\alpha_2} (c_{i,\alpha_1} c_{i,\alpha_2} - c_l^2 \delta_{\alpha_1 \alpha_2})}{2c_l^4}}_{e_{i,nl}^+} + w_i \rho_0 l_{\text{Ma}^4} \mathcal{O}(\text{Ma}^4) + \dots$$

$$e_i^- = w_i \rho_0 \underbrace{\frac{c_{i,\alpha_1} u_{\alpha_1}}{c_l^2}}_{e_{i,1}^-} + w_i \rho_0 l_{\text{Ma}^3} \underbrace{\mathcal{O}(\text{Ma}^3)}_{e_{i,nl}^-} + \dots$$

$$l_{\text{Ma}^j} \in \{0, 1\} \quad \forall j \in \mathbb{N}^+$$



Stokes flow \rightarrow the linear equilibrium (truncation) is sufficient

Navier-Stokes flow \rightarrow we need at least 2nd order expansion.

The values of w_i can be computed in two ways:

- ▶ from the Gauss-Hermite quadrature of the polynomial expansion of the Maxwell-Boltzmann
- ▶ from isotropy conditions.

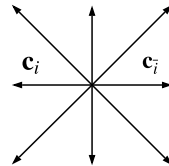
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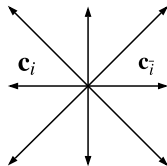
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Solution for the nonequilibrium, Chapman-Enskog + Taylor

Perturbative expansion of f_i :

$$f_{c,i} = e_i + \epsilon f_{c,i}^{(1)} + \epsilon^2 f_{c,i}^{(2)} = e_i + n_{c,i}$$

Perturbative expansion of the operators, assuming diffusive scaling

$$\partial_t = \epsilon^2 \partial_t^{(2)} \quad \partial_\alpha = \epsilon \partial_\alpha^{(1)} + \epsilon^2 \partial_\alpha^{(2)} \quad \forall \alpha \in \{x_1, \dots, x_D\}$$

inject into the (directional) Taylor expansion of the TRT-LBE

$$f_{c,i} + (\epsilon c_{i,\alpha} \partial_\alpha^{(1)} + \epsilon^2 c_{i,\alpha} \partial_\alpha^{(2)} + \epsilon^2 \partial_t^{(2)}) f_{c,i} + (\epsilon c_{i,\alpha} \partial_\alpha^{(1)} + \epsilon^2 c_{i,\alpha} \partial_\alpha^{(2)} + \epsilon^2 \partial_t^{(2)})^2 \frac{f_{c,i}}{2} = f_{c,i} - \frac{n_{c,i}^+}{\tau^+} - \frac{n_{c,i}^-}{\tau^-}.$$

$$\frac{n_{c,i}^\pm}{\tau^\pm} = -c_{i,\alpha} \partial_\alpha e_i^\mp - \partial_t e_i^\pm + \Lambda^\mp (c_{i,\alpha} \partial_\alpha)^2 e_i^\pm, \quad (2)$$

- ▶ The solution is expressed as equilibrium and its derivative;
- ▶ Taking the moments \Rightarrow Navier-Stokes (or Stokes) equations.
- ▶ τ^+ relates with viscosity, τ^- is free for athermal incompressible flows

Directional evolution equation at the boundary

$$\text{LBE: } f_i(\mathbf{x}_{\text{FF}}, t + 1) = \hat{f}_i(\mathbf{x}_{\text{F}}, t + 1)$$

We consider compact or local scheme with max 3 populations (LI or ELI)

Advanced accuracy multireflection schemes need more populations

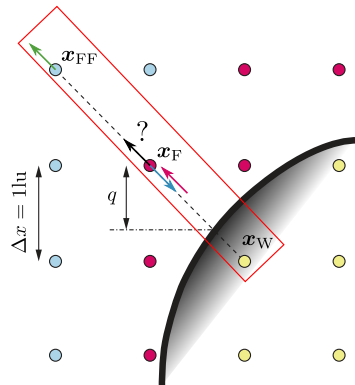
$$f_i(\mathbf{x}_{\text{F}}, t + 1) = \beta \hat{f}_i(\mathbf{x}_{\text{FF}}) + \hat{\alpha} \hat{f}_i(\mathbf{x}_{\text{F}}) + \hat{\beta} \hat{f}_i(\mathbf{x}_{\text{F}}) + \mathcal{E}(\mathbf{x}_{\text{W}}, \bar{t}) + \mathcal{N}(\mathbf{x}_{\text{F}}, t) .$$

$$\mathcal{E}(\mathbf{x}_{\text{W}}, \bar{t}) = -\alpha_e^+ e_i^+(\mathbf{x}_{\text{F}}, t) - \alpha_e^- e_i^-(\mathbf{x}_{\text{F}}, t) - \alpha_{\text{W}}^- e_i^-(\mathbf{x}_{\text{W}}, \bar{t})$$

$$\mathcal{N}(\mathbf{x}_{\text{F}}, t) = \hat{K}^+ \hat{n}_i^+(\mathbf{x}_{\text{F}}, t) + \hat{K}^- \hat{n}_i^-(\mathbf{x}_{\text{F}}, t)$$

📖 LBM directional boundaries: bibliography

Ginzburg and Adler (1994); Ginzburg and d'Humières (2003);
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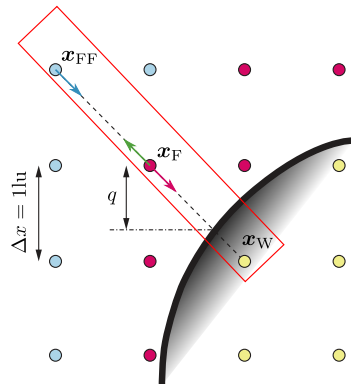
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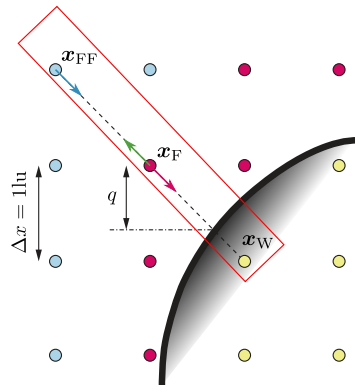
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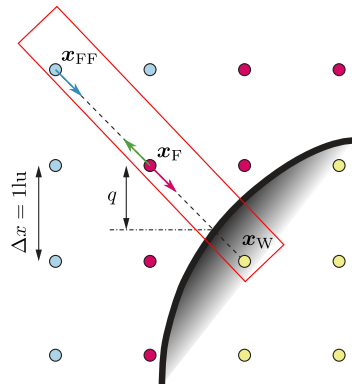
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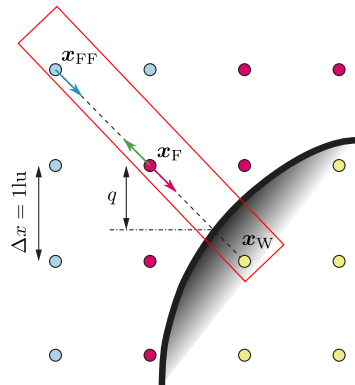
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Uniform formulation: closure

1. Evolution equation at the boundary

$$\left\{ \begin{array}{l} f_i = \beta \hat{f}_i(\mathbf{x}_{FF}) + \hat{\alpha} \hat{f}_i(\mathbf{x}_F) + \hat{\beta} \hat{f}_i(\mathbf{x}_F) \\ \quad + \alpha_\epsilon^+ e_i^+(\mathbf{x}_F) + \alpha_\epsilon^- e_i^-(\mathbf{x}_W) + \alpha_W^- e_i^-(\mathbf{x}_W) \\ \quad - \hat{K}_i^+ \hat{n}_i^+(\mathbf{x}_F) - \hat{K}_i^- \hat{n}_i^-(\mathbf{x}_F) \end{array} \right.$$

 \Leftrightarrow

2. Inject Taylor + CE + '±' decomposition

- ▶ $f_i = e_i + n_i$ equilibrium/nonequilibrium
- ▶ $f_i = e_i^+ + n_i^+ + e_i^- + n_i^-$
- ▶ $n_i = \text{function}(\sum_j \partial^j e_i)$ (Chapman-Enskog)
- ▶ Taylor expansion

💡 Why closure description

The eq. representation \Rightarrow analyze errors introduced by the linear combination.

3. Closure ^a

$$\left[\begin{array}{ll} \alpha^+ e_i^+ & + \alpha^- e_i^- \\ + \beta^+ c_{i,\alpha} \partial_\alpha e_i^+ & + \beta^- c_{i,\alpha} \partial_\alpha e_i^- \\ + \gamma^+ (c_{i,\alpha} \partial_\alpha)^2 e_i^+ & + \gamma^- (c_{i,\alpha} \partial_\alpha)^2 e_i^- \end{array} \right]_{\mathbf{x}_F}^t$$

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$$- \hat{K}_i^+ \hat{n}_i^+(\mathbf{x}_F) - \hat{K}_i^- \hat{n}_i^-(\mathbf{x}_F)$$

linear vel. + linear press. + parabolic vel. & press. + closure corrections + ghost populations

closure coefficients are linear combinations of the “geometrical” ones.

NB α^- are free prefactors: $\alpha^- [f_i^-]_{\mathbf{x}_F} =$

$$\alpha^- \left[f_i^- + q c_{i,\alpha} \partial_\alpha f_i^- + \frac{q^2}{2} (c_{i,\alpha} \partial_\alpha)^2 f_i^- + \dots \right]_{\mathbf{x}_W}$$

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$$= \alpha_\epsilon^+ e_i^+(\mathbf{x}_F) \quad + \alpha_\epsilon^- e_i^-(\mathbf{x}_F) + \alpha_W^- e_i^-(\mathbf{x}_W)$$

$$- \hat{K}_i^+ \hat{n}_i^+(\mathbf{x}_F) \quad - \hat{K}_i^- \hat{n}_i^-(\mathbf{x}_F)$$

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Uniform formulation: closure

1. Evolution equation at the boundary

$$\left\{ \begin{array}{l} f_i = \beta \hat{f}_i(\mathbf{x}_{FF}) + \hat{\alpha} \hat{f}_i(\mathbf{x}_F) + \hat{\beta} \hat{f}_i(\mathbf{x}_F) \\ \quad + \alpha_\epsilon^+ e_i^+(\mathbf{x}_F) \quad + \alpha_\epsilon^- e_i^-(\mathbf{x}_W) + \alpha_W^- e_i^-(\mathbf{x}_W) \\ \quad - \hat{K}_i^+ \hat{n}_i^+(\mathbf{x}_F) \quad - \hat{K}_i^- \hat{n}_i^-(\mathbf{x}_F) \end{array} \right. \iff$$

2. Inject Taylor + CE + '±' decomposition

- ▶ $f_i = e_i + n_i$ equilibrium/nonequilibrium
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The eq. representation \Rightarrow analyze errors introduced by the linear combination.

3. Closure ^a

$$\left[\begin{array}{ll} \alpha^+ e_i^+ & + \alpha^- e_i^- \\ + \beta^+ c_{i,\alpha} \partial_\alpha e_i^+ & + \beta^- c_{i,\alpha} \partial_\alpha e_i^- \\ + \gamma^+ (c_{i,\alpha} \partial_\alpha)^2 e_i^+ & + \gamma^- (c_{i,\alpha} \partial_\alpha)^2 e_i^- \end{array} \right]_{\mathbf{x}_F}^t$$

$$= \alpha_\epsilon^+ e_i^+(\mathbf{x}_F) \quad + \alpha_\epsilon^- e_i^-(\mathbf{x}_F) + \alpha_W^- e_i^-(\mathbf{x}_W)$$

$$- \hat{K}_i^+ \hat{n}_i^+(\mathbf{x}_F) \quad - \hat{K}_i^- \hat{n}_i^-(\mathbf{x}_F)$$

linear vel. + linear press. + **parabolic vel. & press.** +
closure corrections + ghost populations

closure coefficients are linear combinations of the "geometrical" ones.

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Elementary model for narrow gaps: Stokes channel flows

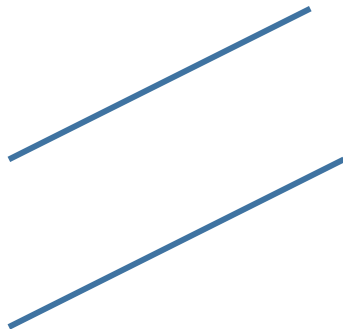
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Analysis of the closure with c/p-flows

- ▶ Identify and cancel errors introduced by the boundary
- ▶ Errors appear sequentially for increasingly complex flows
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 - ⇒ cleaning the right error the elementary flow become exact
- ⇒ accuracy in porous media (Khirevich et al., 2015)

The boundary model is directional ⇒ it is valid for any channel inclination and any complex flow.



s.s. = steady state

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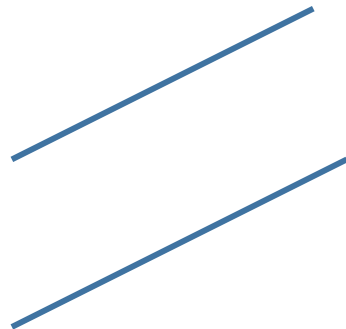
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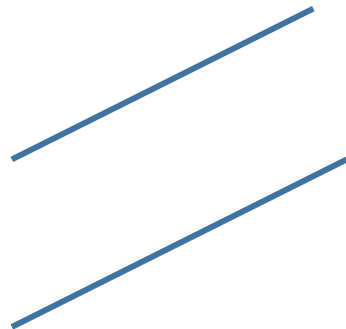
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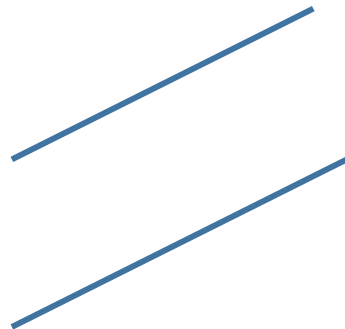
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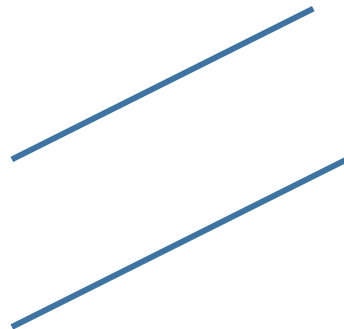
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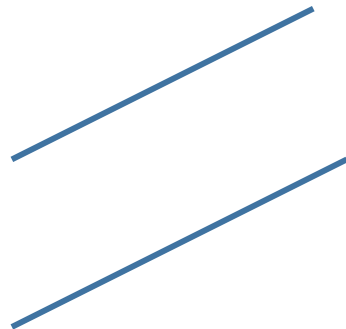
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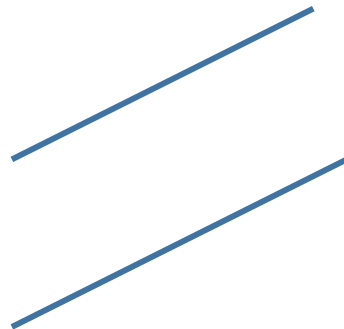
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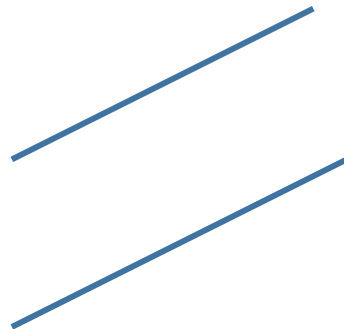
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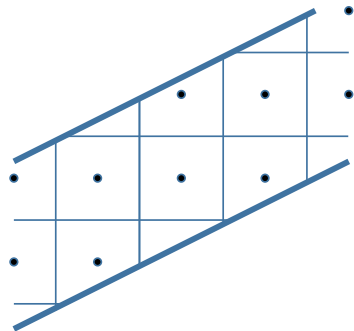
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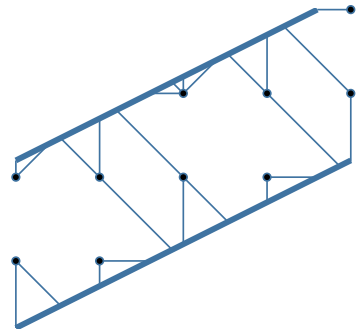
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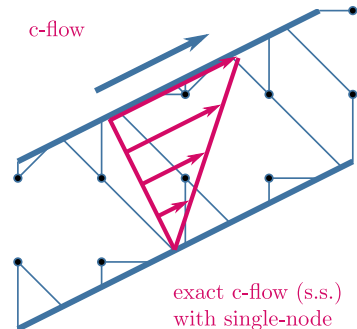
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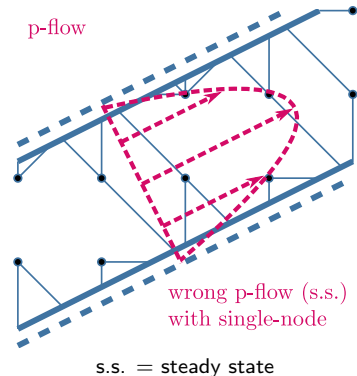
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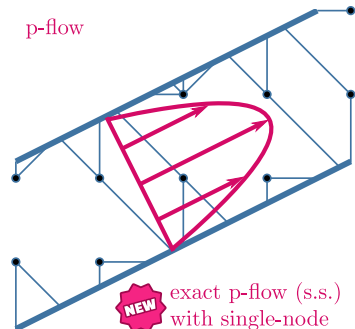
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How to cancel errors locally

Linear case:

$$\alpha^+ = -1 + \hat{\alpha} + \beta + \hat{\beta}$$

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$$\beta^+ = \frac{1}{2}(\hat{\alpha} - \hat{\beta} - \beta - 1) - \alpha^- \Lambda^-$$

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coefficients (errors) depends on Λ^\pm !

Standard (\hat{K}_1^-) correction^a \Rightarrow ELI = LI at s.s.

$$K_1^- \text{ such that } \gamma_K^- \stackrel{\text{def}}{=} \gamma^- - \Lambda^+ \hat{K}^- = \alpha^- \Lambda$$

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New correction \hat{K}_4^- ^c \Rightarrow ELI = LI at s.s.

$$K_4^- \text{ such that } \beta_{\text{tot}}^+ = 0$$

\swarrow linear pressure in Stokes flow!

Resulting single-node schemes are parametrized!

^a  (Ginzburg et al., 2008)

^b  (Marson, 2022; Ginzburg et al., 2022)

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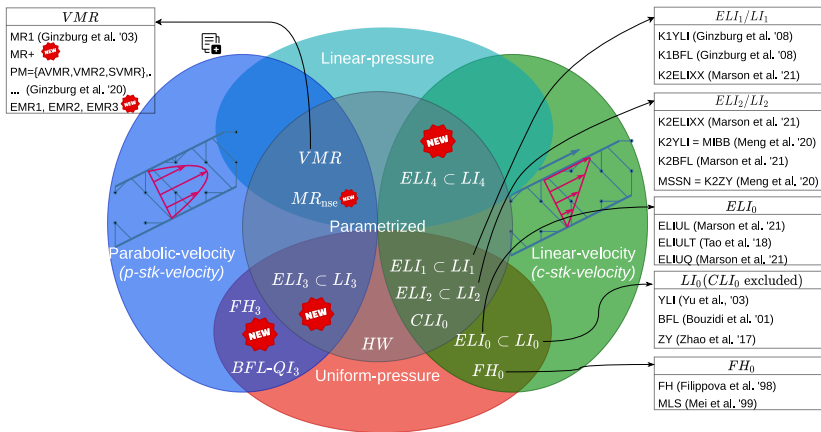
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^c  (Marson, 2022; Ginzburg et al., 2022)

New schemes: Stokes flow classification



(Filippova & Hänel, 1997; Mei et al., 1999; Yu et al., 2003; Ginzburg & d'Humières, 2003; Ginzburg et al., 2008; Marson, Thorimbert, et al., 2021; Zhao & Yong, 2017; Tao et al., 2018; Ginzburg, 2020; Meng et al., 2020; Bouzidi et al., 2001; Marson, Silva, et al., 2021)

Inclined channels

Scheme or Family	Nodes	<i>c-stk-flow</i>	<i>p-stk-flow</i>	param.	<i>c-nse-flow</i>	<i>p-nse-flow</i>
MR _{nse}	3 ~ 4	✓	✓	✓	✓	✓
the parametrized and <i>p-stk-flow</i> schemes						
PM={AVMR, EMR}	2 ~ 3	✓	✓	✓	✓	×
MR={MR1, MR1 ⁺ }	2 ~ 3	✓	✓	✓	×	×
{IPLI, LI ₃ }	1 ~ 2	✓	✓	✓	×	×
{CELI-IP, ELI ₃ }	1	✓	✓	✓	×	×
the parametrized schemes						
LI ₁	1 ~ 2	✓	×	✓	×	×
ELI ₁	1	✓	×	✓	×	×
LI ₄	1 ~ 2	✓	×	✓	×	×
ELI ₄	1	✓	×	✓	×	×
HW	1	×	×	✓	×	×
non-parametrized schemes						
linear-interpolation based:						
LI ₀ ⁺	1 ~ 2	✓	×	×	×	×
ELI ₀	1	✓	×	×	×	×
quadratic-interpolation based:						
BFL-QI ₃	2 ~ 3	✓	✓	×	×	×
BFL-QI	2 ~ 3	✓	×	×	×	×
equilibrium-interpolation based:						
FH ₃	1	✓	✓	×	×	×
FH ₀	1	✓	×	×	×	×
MLS ₃	2	✓	✓	×	×	×
MLS ₀	2	✓	×	×	×	×

Stability optimization

In the bulk

1. collision, with stability condition:

$$\left|1 - 1/\tau^+\right| \leq 1$$

2. streaming.

In the boundary

1. modified collision, with stability condition:

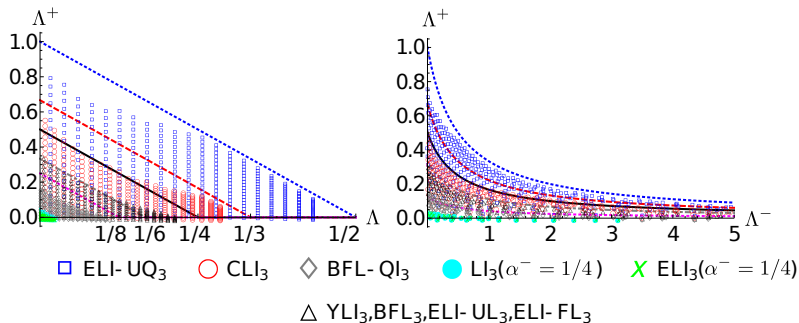
$$\left|1 \mp \beta^\mp / \tau^\pm\right| \leq 1$$

2. modified streaming.

- ▶ accuracy for the steady state solution is the same for all α^- (parametrized schemes);
- ▶ $\beta^- \Rightarrow \alpha^-$ controls the stability proprieties of the schemes!
- ▶ An optimal stability value for $\alpha^-(\Lambda^\pm)$ exists
- ▶ coefficients $\in [-1, 1]$: almost necessary condition, not sufficient with K^-

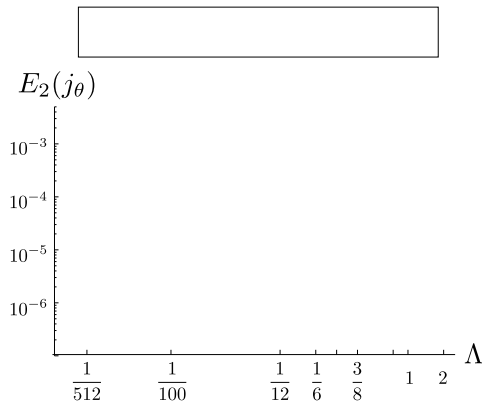
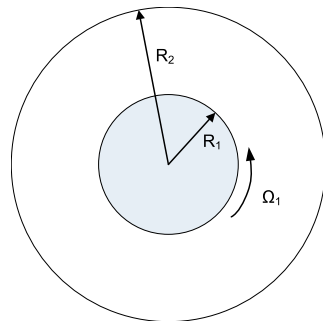
Stability: results

For \hat{K}_3 schemes, the steady state accuracy in p-flow is the same, but stability is different for schemes with different α^-

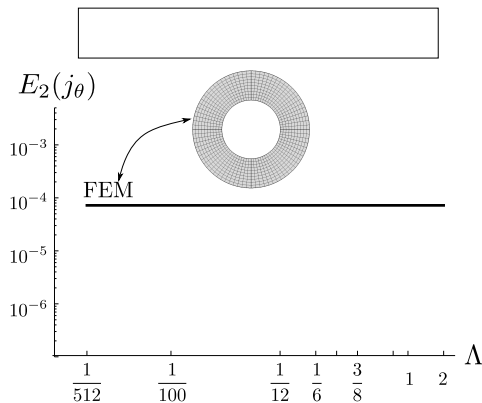
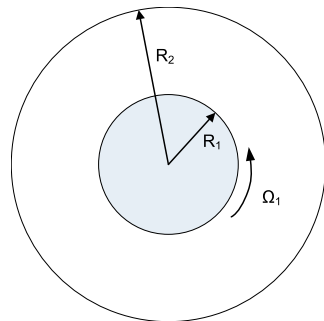


α^- controls the stability properties of the schemes!

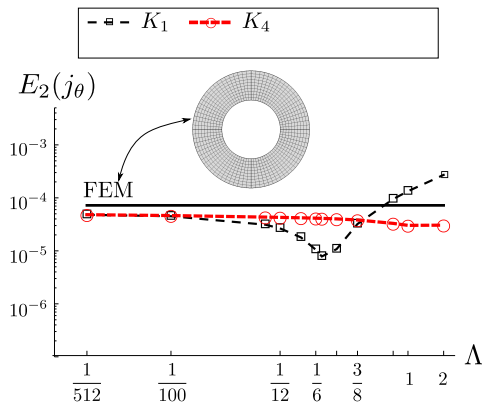
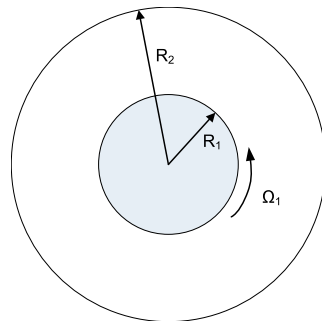
Stokes flow: circular Couette

Figure: $R_2 - R_1 = 10 \text{ lu}$ 

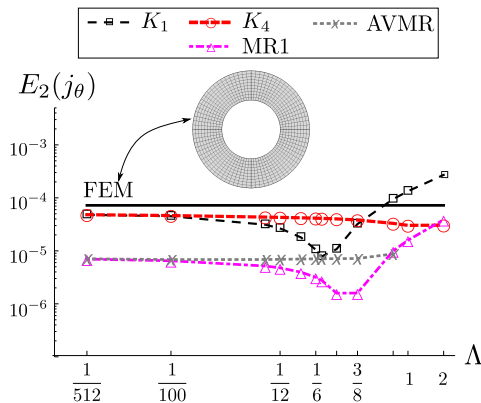
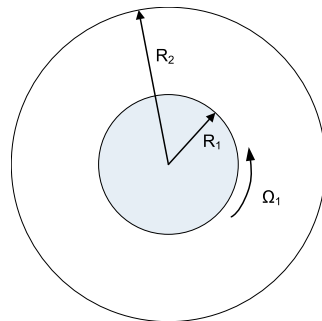
Stokes flow: circular Couette

Figure: $R_2 - R_1 = 10 \text{ lu}$ 

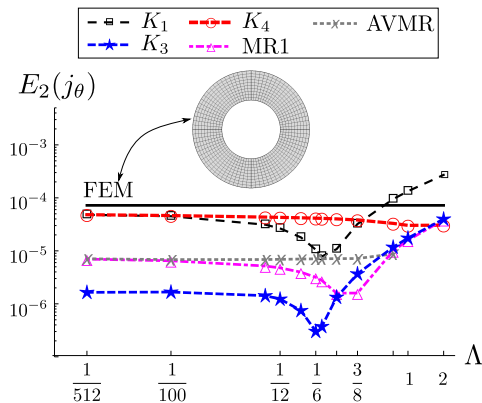
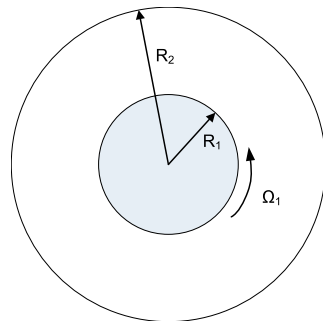
Stokes flow: circular Couette

Figure: $R_2 - R_1 = 10 \text{ lu}$ 

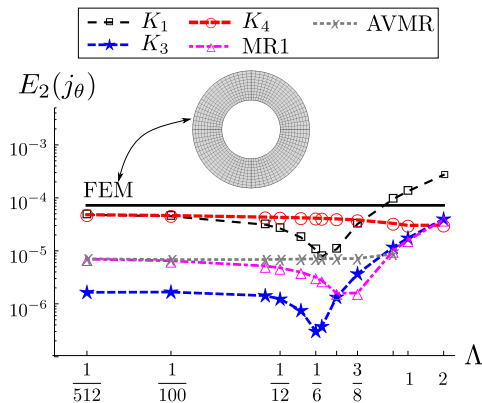
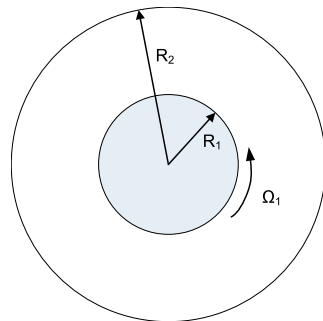
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Figure: $R_2 - R_1 = 10 \text{ lu}$ 

Stokes flow: circular Couette

Figure: $R_2 - R_1 = 10 \text{ lu}$ 

Stokes flow: circular Couette

Figure: $R_2 - R_1 = 10 \text{ lu}$ 

Stokes flow: results in arrays

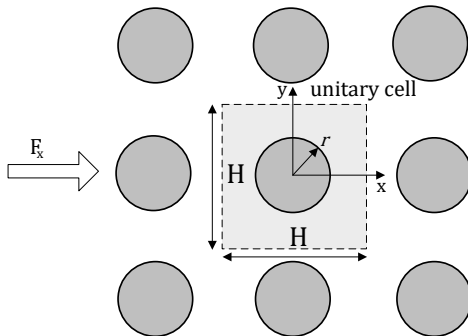


Figure: Schematic representation of the simulation domain for the array of cylinders configuration (Silva, 2018).

Stokes flow: results in arrays

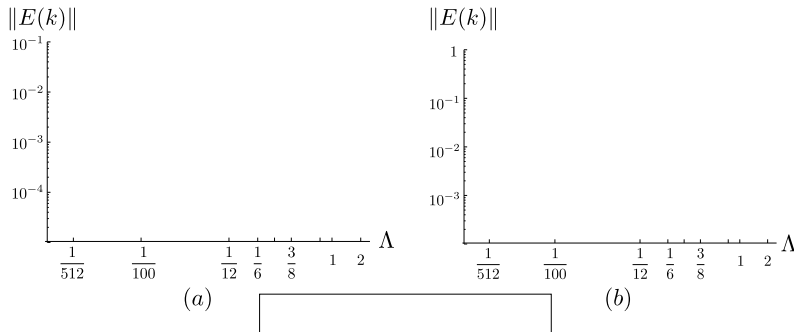



Figure: Permeability estimation error in an array of cylinders using darcy law. (a) and (b): dilute flow with solid fraction $c = 0.2$. (a) cell resolution $H^2 = 33^2 \text{ lu}^2$. (b) cell resolution $H^2 = 99^2 \text{ lu}^2$.

 (Ginzburg et al., 2022; Marson, 2022)

Stokes flow: results in arrays

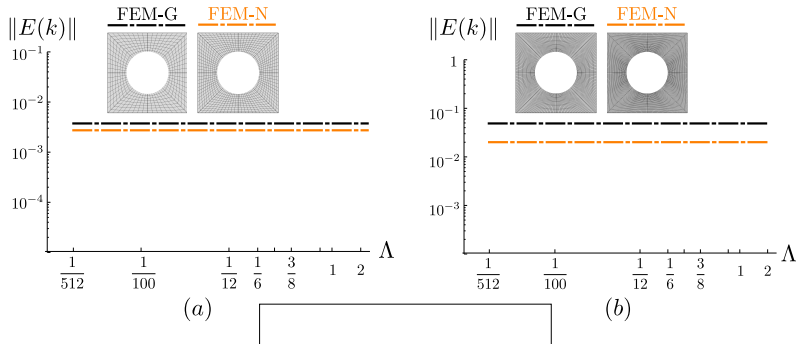


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📖 (Ginzburg et al., 2022; Marson, 2022)

Stokes flow: results in arrays

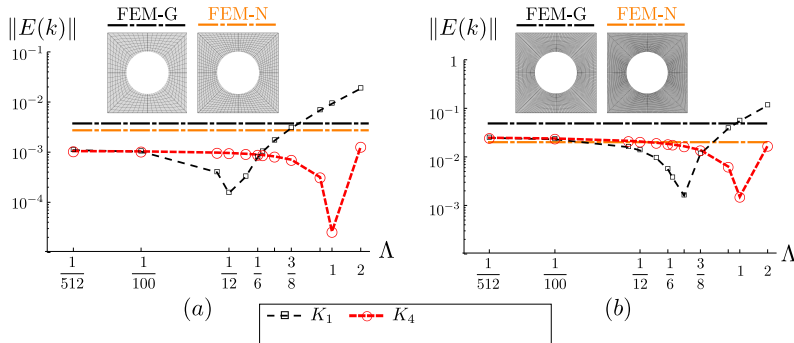


Figure: Permeability estimation error in an array of cylinders using darcy law. (a) and (b): dilute flow with solid fraction $c = 0.2$. (a) cell resolution $H^2 = 33^2 \text{ lu}^2$. (b) cell resolution $H^2 = 99^2 \text{ lu}^2$.

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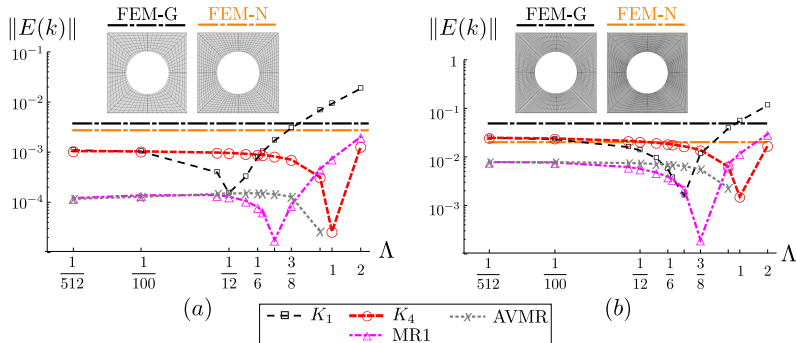



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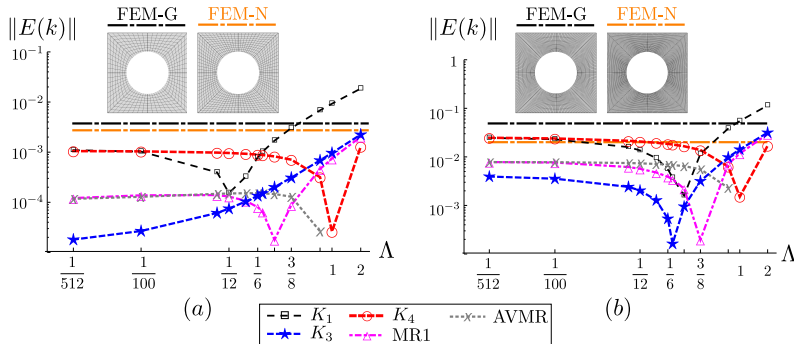

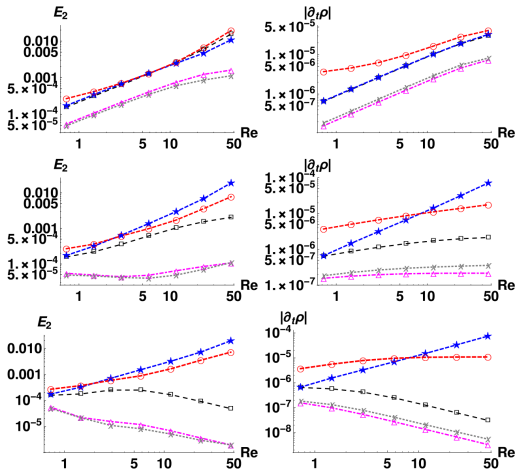


Figure: Permeability estimation error in an array of cylinders using darcy law. (a) and (b): dilute flow with solid fraction $c = 0.2$. (a) cell resolution $H^2 = 33^2 \text{ lu}^2$. (b) cell resolution $H^2 = 99^2 \text{ lu}^2$.

 (Ginzburg et al., 2022; Marson, 2022)

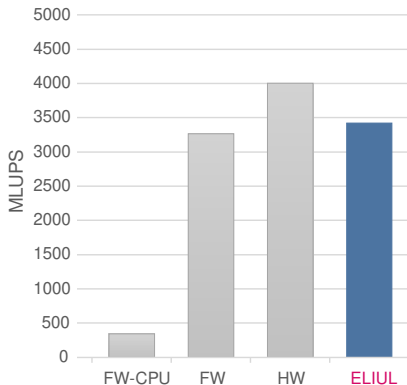
Finite Re

Error as a function of **grid** Reynolds $Re = u_{lb}/\nu_{lb}$



- ▶ LBE with standard NSE equilibrium \rightarrow inexact solutions for c/p -nse-flows
- ▶ higher order errors appear in the closure
- ▶ results are non-parametrized
- ▶ find optimal scaling for $\Lambda = \Lambda^+ \Lambda^-$

Sandstone porous medium with Palabos on GPUs



Sandstone porous medium
MLUPS = Million Lattice Updates Per Second

Thank you! Questions?



THANK YOU FOR YOUR ATTENTION! QUESTIONS?

Acknowledgments



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PALABOS

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