Westfälische
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Applying Volume Penalization Methods to Turbulent Rayleigh-Bénard Convection

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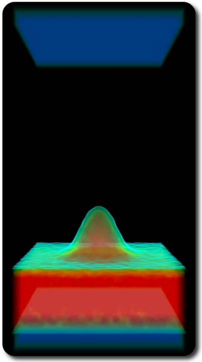

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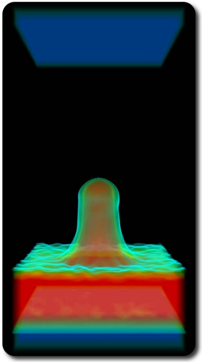
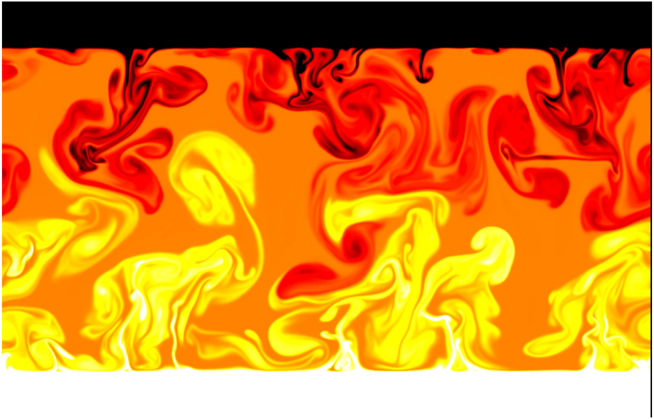


- Boundaries

Importance of boundaries[o]



[o] Videos of this talk to be found at `www.youtube.com/turbulenceteamms`

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Importance of boundaries

- Every real system has boundaries
- Important effects near boundaries
  $\rightarrow$ Boundary layers, ...
- Analytical analysis difficult or impossible
  $\rightarrow$ Neglection of boundaries
- Numerical simulation possible, but often difficult

$\Rightarrow$ Develop **easy-to-use** and **flexible** numerical methods

Contents

Pseudospectral Method for Navier-Stokes equation

Navier-Stokes Equation

$$\frac{\partial}{\partial t}\mathbf{u}(\mathbf{x},t) + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t) = -\nabla p(\mathbf{x},t) + \nu\Delta\mathbf{u}(\mathbf{x},t)$$
$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0$$

- Nonlinear
- Nonlocal
- Unsolvable

Pseudospectral Method for Navier-Stokes equation

Fourier Transformation

- Linear integral transformation:

$$\widetilde{g}(\mathbf{k}) = \mathcal{F}\left[g(\mathbf{x})\right](\mathbf{k}) = \frac{1}{\sqrt{2\pi}^3} \int \mathrm{d}^3x \, g(\mathbf{x}) \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$g(\mathbf{x}) = \mathcal{F}^{-1}\left[\widetilde{g}(\mathbf{k})\right](\mathbf{x}) = \frac{1}{\sqrt{2\pi}^3} \int \mathrm{d}^3k \, \widetilde{g}(\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

Fourier Transformation of Derivative

$$\mathcal{F}\left[\nabla g(\mathbf{x})\right](\mathbf{k}) = \mathrm{i}\mathbf{k}\,\mathcal{F}\left[g(\mathbf{x})\right](\mathbf{k}) = \mathrm{i}\mathbf{k}\,\widetilde{g}(\mathbf{k})$$

Pseudospectral Method for Navier-Stokes equation

Navier-Stokes Equation for $\widetilde{\mathbf{u}}(\mathbf{k}, t) = \mathcal{F}\left[\mathbf{u}(\mathbf{x}, t)\right](\mathbf{k}, t)$

$$\frac{\partial}{\partial t}\widetilde{\mathbf{u}} + \mathcal{F}\left[\mathbf{u} \cdot \nabla \mathbf{u}\right] = \mathcal{F}\left[-\nabla p\right] - \nu \mathbf{k}^2 \widetilde{\mathbf{u}}$$

- How to express $\mathcal{F}\left[\mathbf{u} \cdot \nabla \mathbf{u}\right]$ and $\mathcal{F}\left[-\nabla p\right]$ in terms of $\widetilde{\mathbf{u}}$?

Pseudospectral Method for Navier-Stokes equation

Dealing with the Nonlinearity $\mathbf{u} \cdot \nabla \mathbf{u}$

- Instead of convolution in Fourier Space

$$\mathcal{F}\left[\mathbf{u} \cdot \nabla \mathbf{u}\right] = \widetilde{\mathbf{u}} * (\mathrm{i}\mathbf{k}\widetilde{\mathbf{u}})$$

calculate nonlinearity in Real Space:

$$\mathcal{F}\left[\mathbf{u} \cdot \nabla \mathbf{u}\right] = \mathcal{F}\left[\mathcal{F}^{-1}\left[\widetilde{\mathbf{u}}\right] \cdot \mathcal{F}^{-1}\left[\mathrm{i}\mathbf{k}\widetilde{\mathbf{u}}\right]\right]$$

Pseudospectral Method for Navier-Stokes equation

Dealing with the Nonlocality $-\nabla p$

- Since $\nabla \cdot \mathbf{u} = 0$:

$$-\nabla p = \nabla \Delta^{-1} \nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u})$$

- In Fourier Space:

$$\begin{aligned} \mathcal{F}[-\nabla p] &= \frac{\mathbf{kk}}{\mathbf{k}^2} \mathcal{F}[\mathbf{u} \cdot \nabla \mathbf{u}] \\ &= \frac{\mathbf{kk}}{\mathbf{k}^2} \mathcal{F}\left[\mathcal{F}^{-1}\left[\widetilde{\mathbf{u}}\right] \cdot \mathcal{F}^{-1}\left[i\mathbf{k}\widetilde{\mathbf{u}}\right]\right] \end{aligned}$$

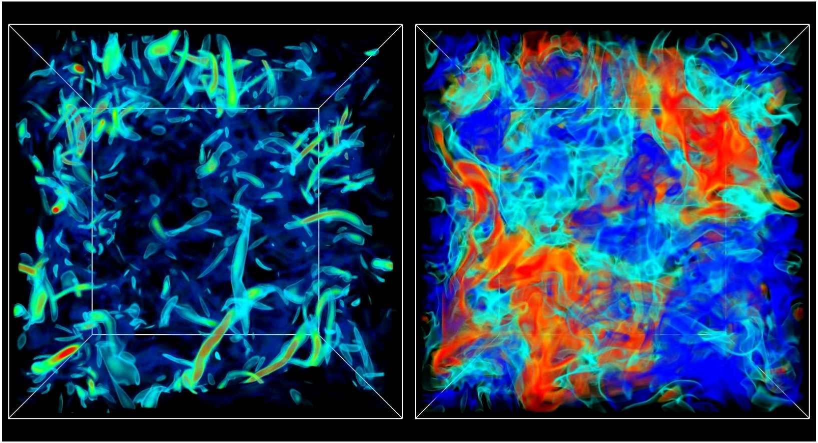
Pseudospectral Method for Navier-Stokes equation

Navier-Stokes Equation in Pseudospectral Form

$$\frac{\partial}{\partial t}\widetilde{\mathbf{u}} = -\left(\mathrm{E}_3 - \frac{\mathbf{k}\mathbf{k}}{\mathbf{k}^2}\right)\mathcal{F}\left[\mathcal{F}^{-1}\left[\widetilde{\mathbf{u}}\right]\cdot\mathcal{F}^{-1}\left[\mathrm{i}\mathbf{k}\widetilde{\mathbf{u}}\right]\right] - \nu\mathbf{k}^2\widetilde{\mathbf{u}}$$

- Set of Ordinary Differential Equations for $\widetilde{\mathbf{u}} = \widetilde{\mathbf{u}}(\mathbf{k}, t)$
  $\rightarrow$ Discretize $\mathbf{u}$ resp. $\widetilde{\mathbf{u}}$ on grid
  $\rightarrow$ Solve ODE numerically with timestepping scheme!

Pseudospectral Method for Navier-Stokes equation



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Volume Penalization

Boundary Conditions

- Up to now: periodic boundaries
- How to implement solid walls, i.e. no slip boundaries, into the pseudospectral method?

The Idea behind Volume Penalization

- Separate the periodic volume into fluid regions and wall regions via masking function $H(\mathbf{x}) \in \{0, 1\}$
- In the wall parts, add strong damping term to Navier-Stokes equation that models walls

Volume Penalization

Damping Term the Easy Way

$$\frac{\mathrm{d}}{\mathrm{d}t} y(x,t) = -\frac{1}{\eta} H(x) y(x,t)$$
$$\Rightarrow y(x,t) = y(x,0)\, \mathrm{e}^{-\frac{1}{\eta} H(x) t}$$

In the different regions:

- $H(x) = 0$: y remains unchanged: $y(x,t) = y(x,0)$
- $H(x) = 1$: y is exponentially damped:
  $\lim_{t \to \infty} y(x,t) = \lim_{\eta \to 0} y(x,t) = 0$

Volume Penalization

Volume Penalized Navier-Stokes Equation[1]

$$\frac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\Delta\mathbf{u} - \frac{1}{\eta}H\cdot\mathbf{u}$$
$$\nabla\cdot\mathbf{u} = 0$$

- $\eta \ll 1$: Penalization Parameter

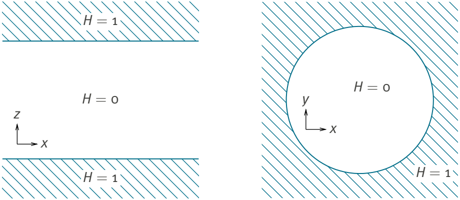
[1] e.g.: Kai Schneider. Numerical simulation of the transient flow behaviour in chemical reactors using a penalisation method. *Computers & Fluids*, 34(10):1223–1238, 2005.

Volume Penalization

Volume Penalized Navier-Stokes Equation in Fourier Space

$$\frac{\partial}{\partial t}\widetilde{\mathbf{u}} = -\left(\mathrm{E}_3 - \frac{\mathbf{k}\mathbf{k}}{\mathbf{k}^2}\right)\mathcal{F}\left[\mathcal{F}^{-1}\left[\widetilde{\mathbf{u}}\right]\cdot\mathcal{F}^{-1}\left[\mathrm{i}\mathbf{k}\widetilde{\mathbf{u}}\right]\right] - \nu\mathbf{k}^2\widetilde{\mathbf{u}}$$
$$-\frac{1}{\eta}\mathcal{F}\left[H(\mathbf{x})\cdot\mathcal{F}^{-1}\left[\widetilde{\mathbf{u}}\right]\right]$$

Volume Penalization

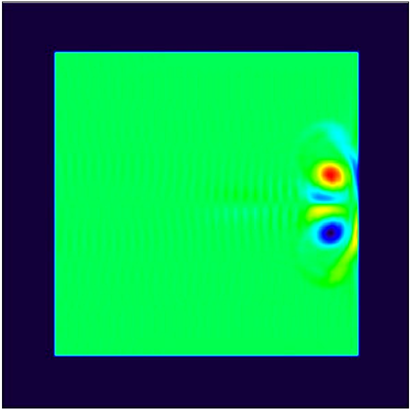


- Boundary conditions converge[2] to no slip boundaries for $\eta \to 0$
- Convenient choice for η: Dependent on numerical resolution![3]

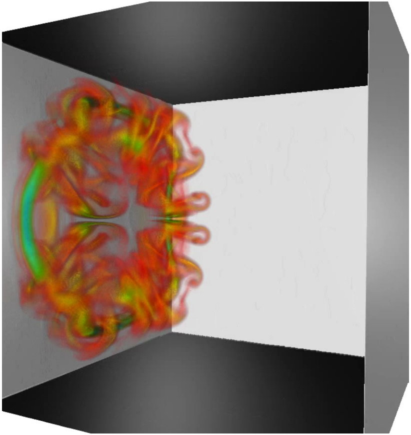
[2] P. Angot, C.-H. Bruneau, and P. Fabrie. *Numerische Mathematik*, 81(4):497–520, 1999.

[3] G. H. Keetels et al. *Journal of Computational Physics*, 227(2):919–945, 2007.

Volume Penalization



Volume Penalization



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Application to Convection

Oberbeck-Boussinesq Equations

$$\frac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \mathrm{Pr}\Delta\mathbf{u} + \mathrm{Pr}\,\mathrm{Ra}\,T\mathbf{e}_z \quad , \quad \nabla\cdot\mathbf{u} = 0$$

$$\frac{\partial}{\partial t}T + \mathbf{u}\cdot\nabla T = \Delta T$$

Boundary Conditions

$$\mathbf{u}(z{=}0) = \mathbf{u}(z{=}1) = 0$$

$$T(z{=}0) = {}^1\!/_2$$

$$T(z{=}1) = -{}^1\!/_2$$

Application to Convection

- No slip boundaries for velocity field $\rightarrow$ straightforward!
- Plates of constant temperature $\rightarrow$ variable change![4]

Deviation from Linear Temperature Profile

$$\theta(\mathbf{x}, t) = T(\mathbf{x}, t) + \left(z - \frac{1}{2}\right)$$

New Boundary Conditions

$$\theta(z=0) = \theta(z=1) = 0$$

[4] JL. Statistische Eigenschaften turbulenter Rayleigh-Bénard-Konvektion. Diplomarbeit, Westfälische Wilhelms-Universität Münster, 2011.

Application to Convection

- Boundary conditions for θ can be achieved via Volume Penalization!

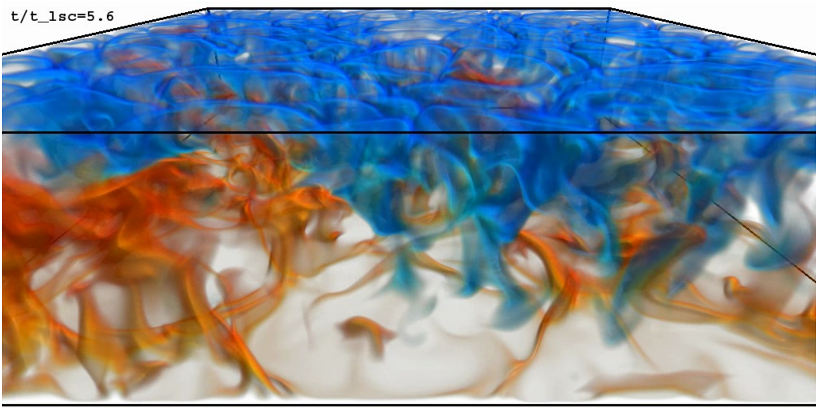
Volume Penalized Oberbeck-Boussinesq Equations

$$\frac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\Delta\mathbf{u} + \mathrm{Pr}\,\mathrm{Ra}\,T\mathbf{e}_z - \frac{1}{\eta}H\cdot\mathbf{u}$$

$$\nabla\cdot\mathbf{u} = 0$$

$$\frac{\partial}{\partial t}\theta + \mathbf{u}\cdot\nabla\theta = \Delta\theta + \mathbf{u}\cdot\mathbf{e}_z - \frac{1}{\eta}H\cdot\theta$$

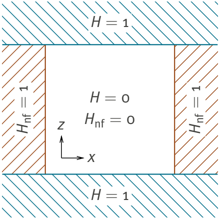
Application to Convection



Application to Convection

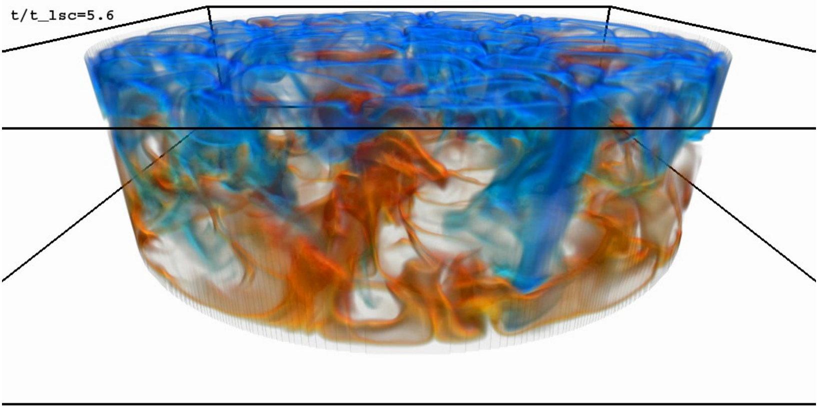
Application to Convection – Insulating Sidewalls

- Up to now: Dirichlet boundaries, i.e. fixed temperature, also for sidewalls
- Extension to insulating sidewalls, i.e. von Neumann boundaries, possible![5]

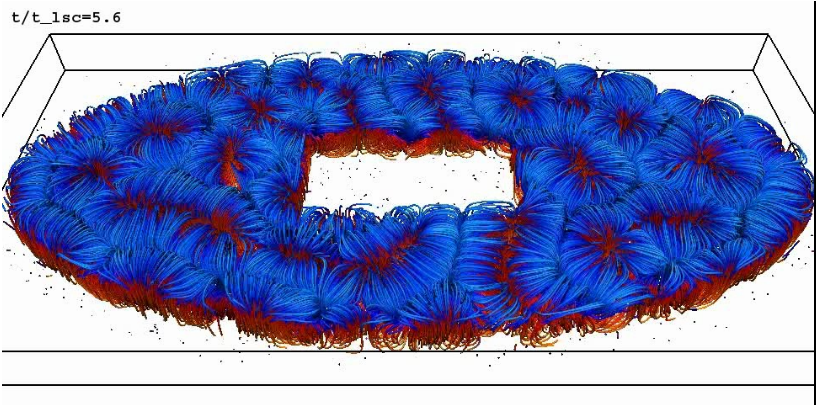


[5]JL. Statistische Eigenschaften turbulenter Rayleigh-Bénard-Konvektion. Diplomarbeit, Westfälische Wilhelms-Universität Münster, 2011.

Application to Convection – Insulating Sidewalls



Application to Convection – Insulating Sidewalls



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Implementation and Results

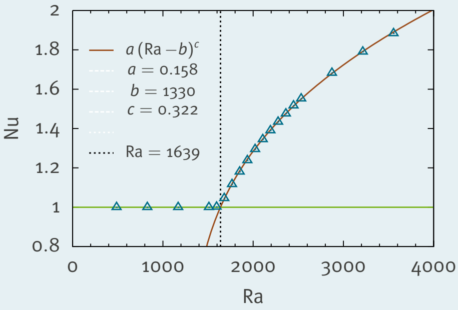
Implementation Details

- 3D pseudospectral code with tri-periodic boundaries and dealiasing[6]
- Fast Fourier Transformations provided by FFTW[7]
- Timestepping by RK3 method[8] with *integrating factor*
- Parallelization via MPI slab decomposition facilitated by FFTW

[6] Thomas Y. Hou and Ruo Li. *J. Comp. Phys.*, 226:379–397, 2007
[7] `www.fftw.org`
[8] Chi-Wang Shu and Stanley Osher. *J. Comp. Phys.*, 77(2):439–471, 1988

Implementation and Results

Statistical Validation of Numerics



- $\mathrm{Ra}_c = 1707.9 \;\rightarrow\; \dfrac{\mathrm{Ra}_c - \mathrm{Ra}}{\mathrm{Ra}_c} < 5\%$

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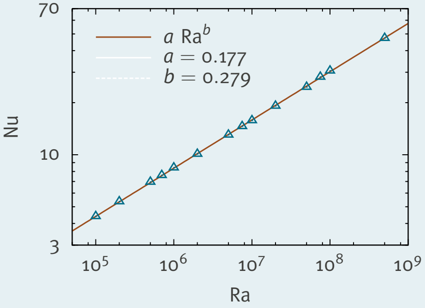
Implementation and Results

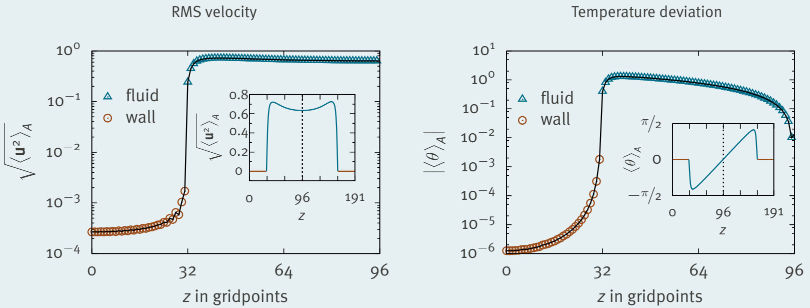
Statistical Validation of Numerics



- Literature: Nu $\sim$ Ra$^{2/7}$ $\approx$ Ra$^{0.286}$

Implementation and Results

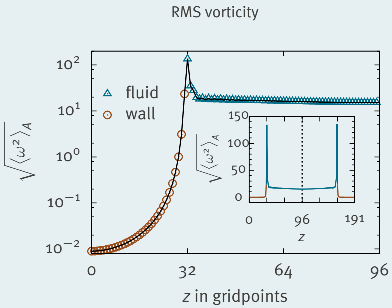
Pointwise Validation of Numerics ($\mathrm{Ra} = 2.4 \times 10^8, \eta = 10^{-3}$)

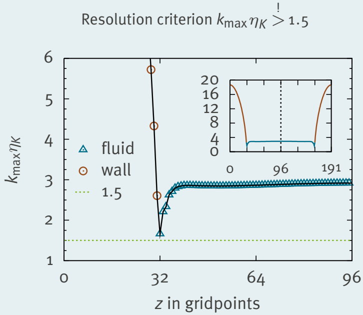


- Jump over ~ 2.5 orders of magnitude between fluid and wall

Implementation and Results

Pointwise Validation of Numerics ($\mathrm{Ra} = 2.4 \times 10^8$, $\eta = 10^{-3}$)





- Resolution of boundary layers is critical!

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Discussion

Upsides

- Arbitrary wall shapes possible
- Walls are easy to design
- Trivial extension of the basic equations
  $\rightarrow$ Easy to implement
  $\rightarrow$ Easy to incorporate into existing numerics
- Fast ($\rightarrow$ 'pseudospectral fast')

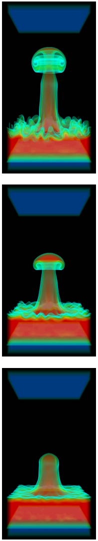
Discussion

Downsides

- Discontinuous masking function: Gibbs oscillations occur near surfaces!
  $\rightarrow$ not dynamically active, can be filtered in post processing
  $\rightarrow$ Smoothing of masking function
- Numerical scheme becomes stiff: limit $\eta \rightarrow 0$ technical difficult!
  $\rightarrow$ Implicit treatment of penalization term possible
- When implemented as extension of pseudospectral codes: no clustering of gridpoints, resolution problems!
  $\rightarrow$ Implement Volume Penalization as extension of other numerical schemes (e.g. Chebyshev methods)
- Overhead due to wall regions

Conclusion

- Boundaries: They are everywhere!
- Pseudospectral method: Exact evaluation of derivatives in Fourier Space, calculation of nonlinearities in Real Space. Downside: periodic boundaries!
- Volume Penalization: Separation of simulation volume into fluid and wall regions, strong exponential damping applied to wall regions
- Application to Convection: Variable change Temperature→Temperature deviation, insulating sidewalls possible
- Upside: Easy and fast, flexible
- Downside: (Solvable) technical difficulties, overhead



Thank you for your attention!

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Center for Nonlinear Science

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2 Philippe Angot, Charles-Henri Bruneau, and Pierre Fabrie. A penalization method to take into account obstacles in incompressible viscous flows. *Numerische Mathematik*, 81(4):497–520, Feb 1999.

3 G. H. Keetels, U. D'Ortona, W. Kramer, H. J. H. Clercx, K. Schneider, and G. J. F. van Heijst. Fourier spectral and wavelet solvers for the incompressible Navier-Stokes equations with volume-penalization: Convergence of a dipole-wall collision. *Journal of Computational Physics*, 227(2):919–945, 2007.

4,5 Johannes Lülff. *Statistische Eigenschaften turbulenter Rayleigh-Bénard-Konvektion*. Diplomarbeit, Westfälische Wilhelms-Universität Münster, Jan 2011.

6 Thomas Y. Hou and Ruo Li. Computing nearly singular solutions using pseudo-spectral methods. *Journal of Computational Physics*, 226:379–397, Apr 2007.

8 Chi-Wang Shu and Stanley Osher. Efficient implementation of essentially non-oscillatory shock-capturing schemes. *Journal of Computational Physics*, 77(2):439–471, 1988.

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