Analysis of the Large-Scale Order in Turbulent Mesoscale Convection

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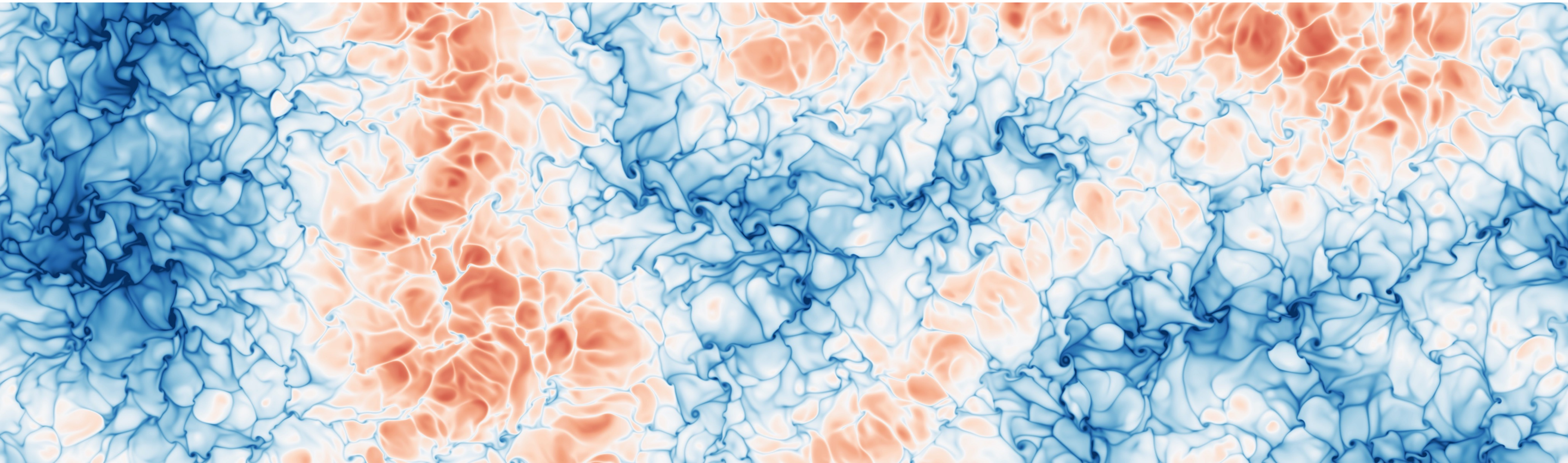
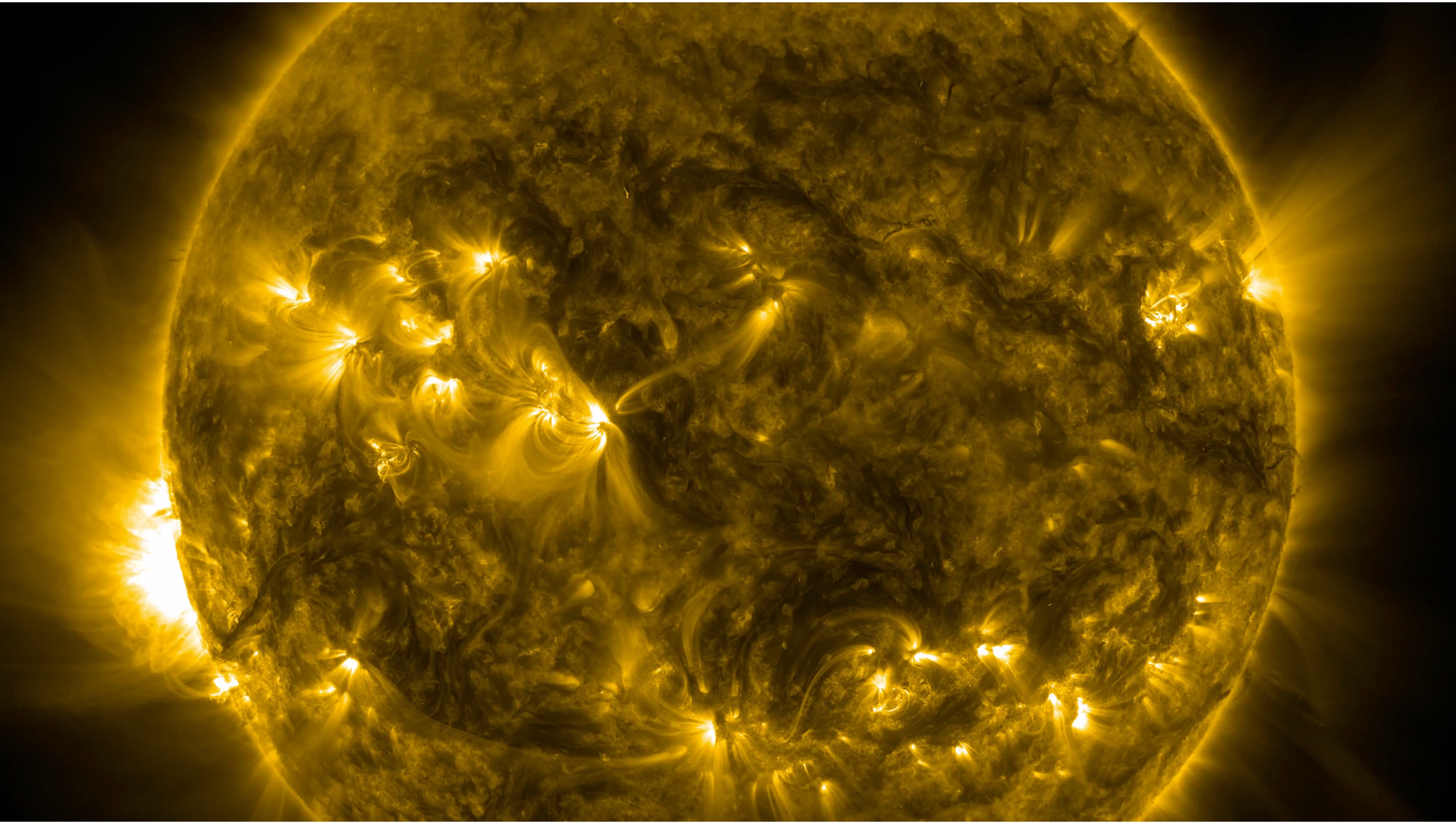


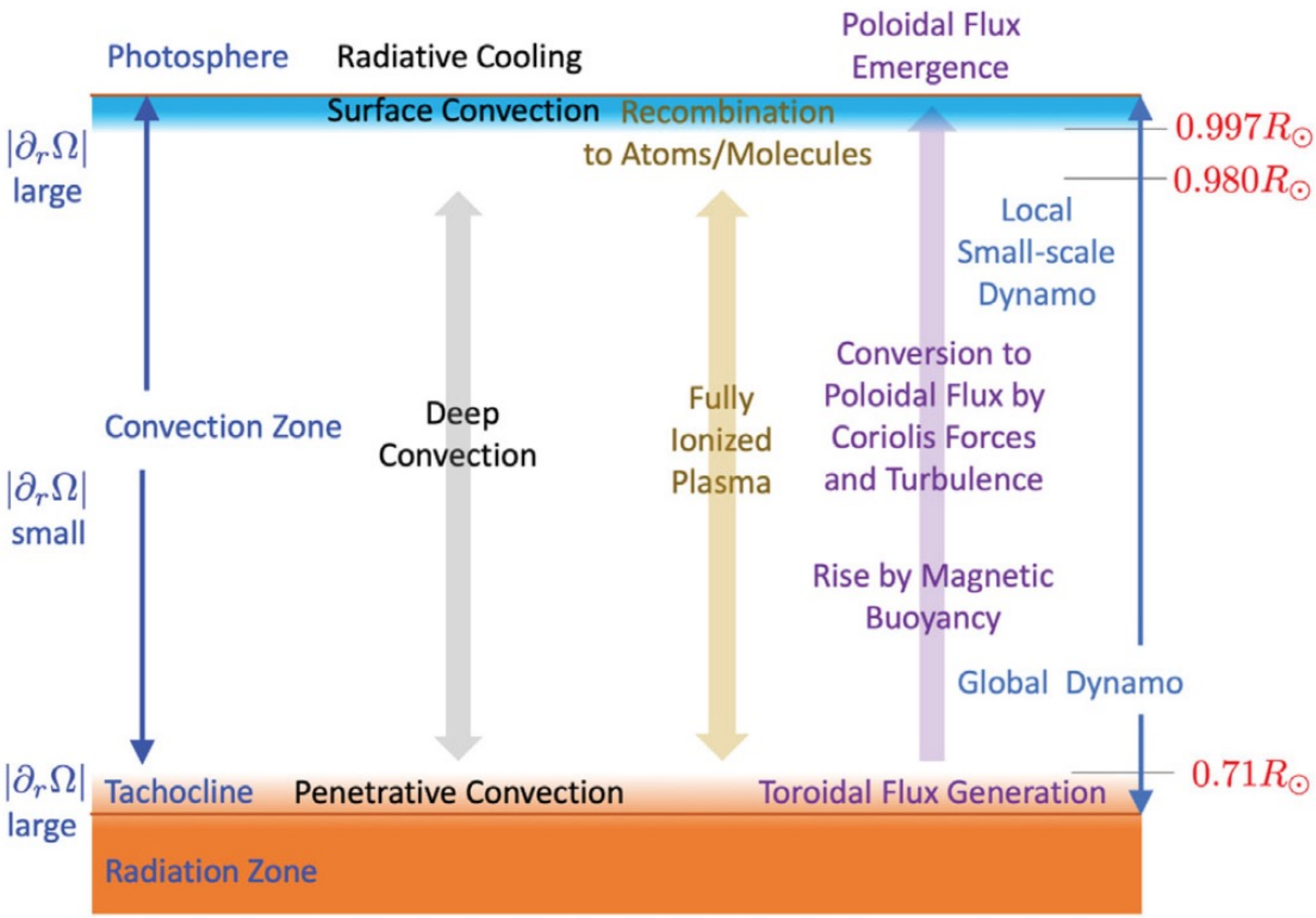
The Sun



Courtesy of Hannah Schunker, MPI for Solar System Research, Göttingen

Convective turbulence in the Sun

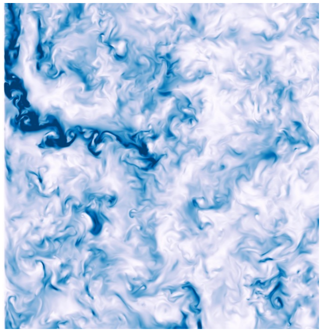
*JS and K.R. Sreenivasan, Rev. Mod. Phys. **92**, 041001 (2020)*



$$\mathrm{Ra} \sim 10^{22} \quad \mathrm{Pr} \sim 10^{-6}$$

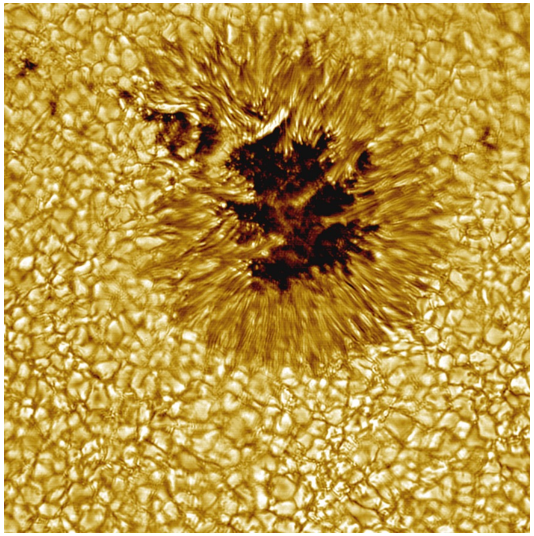
Mesoscale convection

Small Scales
$< 10^2$ km

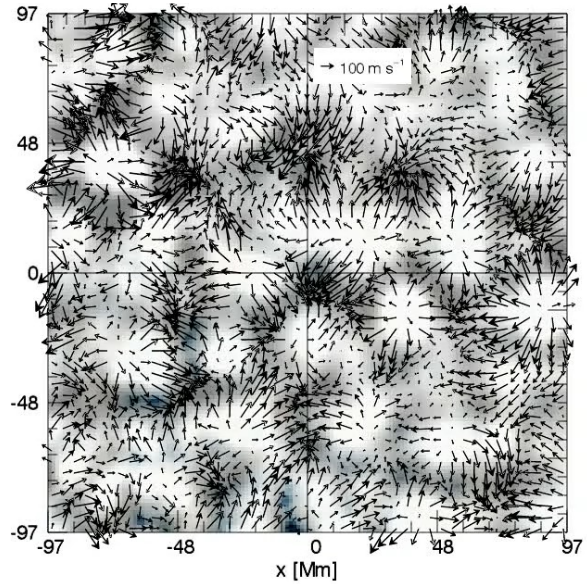


Mesoscales

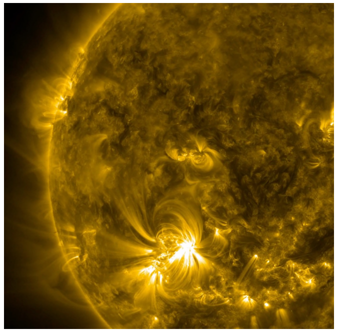
nasa.gov



*Schunker et al., A & A **625**, A53 (2019)*



Global Scales
$> 10^5$ km



	Granules	Supergranules
Scale	1,000 km	30,000 km
Lifetime	10 min	24 h
Velocity	3 km/s	500 m/s
Observation	Optical	Helioseismology or Granule Tracking

Outline

Can we understand and model this order at the mesoscale in simpler models of convection?

- Role of boundary conditions at top/bottom of convection layer
- Effect of additional slow rotation
- Very low Prandtl numbers in convection
- Extension to compressible (top-down symmetry breaking) convection
- Data reduction by classical and quantum machine learning

Florian Heyder (TU Ilmenau)
Dmitry Krasnov (TU Ilmenau)
Juan Pedro Mellado (University of Hamburg)
Ambrish Pandey (New York University Abu Dhabi→IIT Roorkee)
John Panickacheril John (TU Ilmenau)
Philipp Pfeffer (TU Ilmenau)
Janet D. Scheel (Occidental College Los Angeles)
Katepalli R. Sreenivasan (New York University
Rodion Stepanov (Institute of Mechanics Perm)
Philipp P. Vieweg (TU Ilmenau)

- Role of boundary conditions
- Effect of additional rotation
- Very low Prandtl numbers
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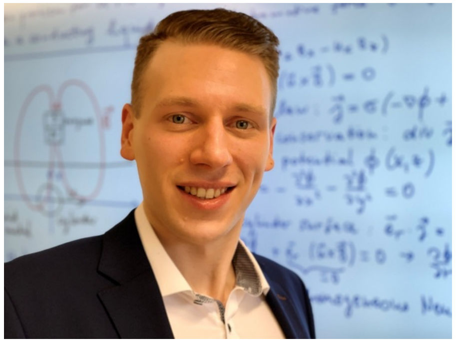


P.P. Vieweg

Rayleigh-Bénard model

Mass balance

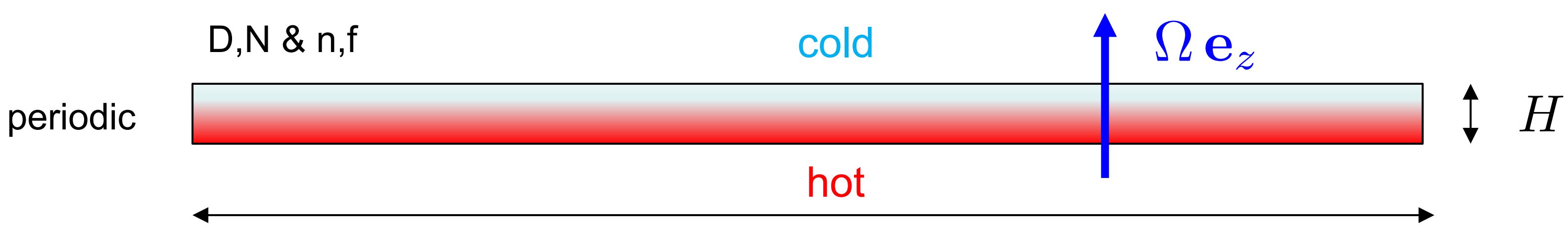
$$\nabla \cdot \boldsymbol{u} = 0\,,$$

Momentum balance

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \frac{1}{\mathrm{Ro}}\boldsymbol{e}_z \times \boldsymbol{u} = -\nabla p + \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}_{D,N}}}\nabla^2 \boldsymbol{u} + T\boldsymbol{e}_z\,,$$

Energy balance

$$\frac{\partial T}{\partial t} + (\boldsymbol{u}\cdot\nabla)T = \frac{1}{\sqrt{\mathrm{Ra}_{D,N}\mathrm{Pr}}}\nabla^2 T\,,$$



$$L_x = L_y = 60H$$

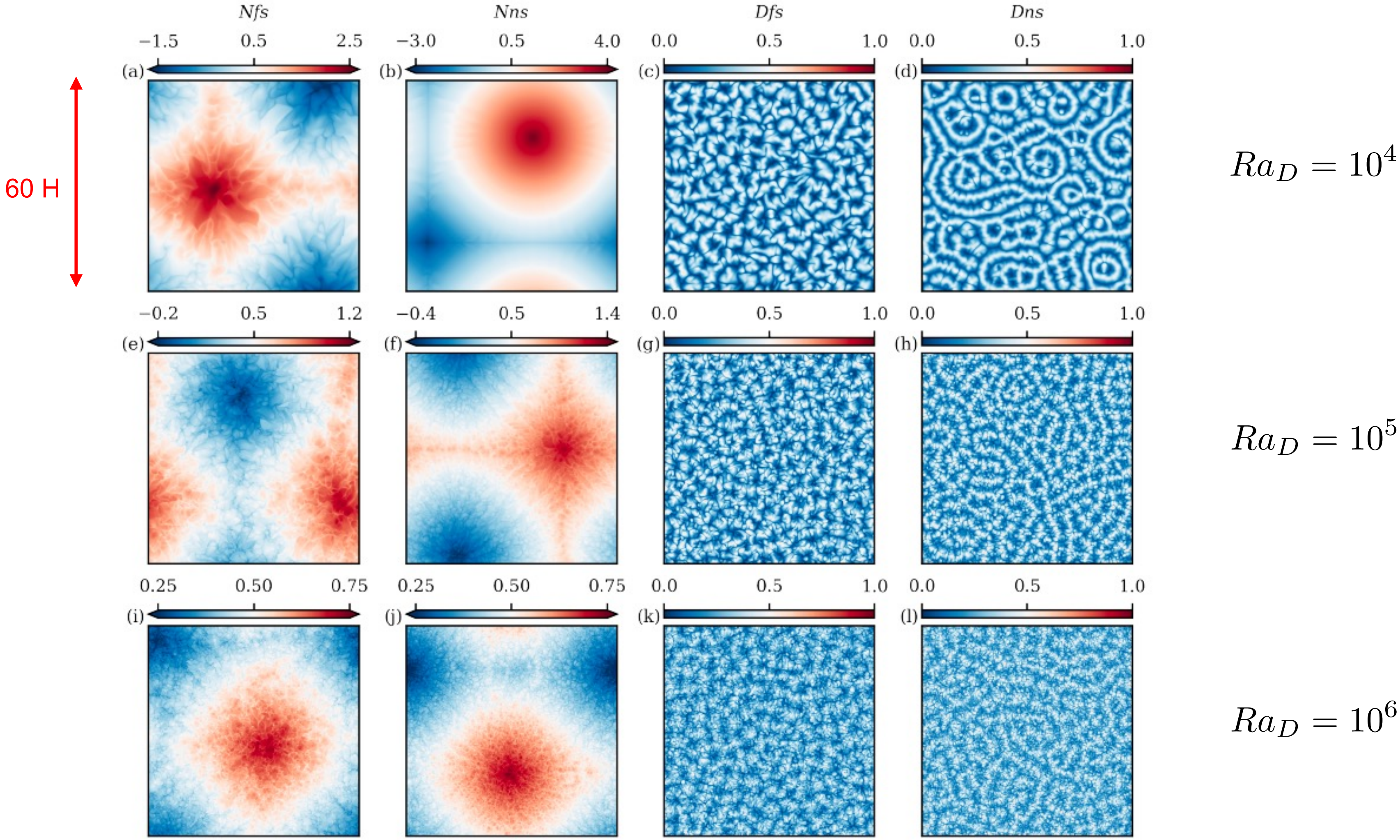
$$\mathrm{Pr} = \frac{\nu}{\kappa} = 1 \qquad \mathrm{Ra}_D = \frac{g\alpha\Delta T H^3}{\nu\kappa} \qquad \mathrm{Ra}_N = \frac{g\alpha\beta H^4}{\nu\kappa} \qquad \mathrm{Ro} = \frac{U_f}{2\Omega H} \gtrsim 1$$

D=Dirichlet (set temperature value)
N=Neumann (set temperature derivative)

f=free-slip (flow slips along planes)
n=no-slip (flow stucks at planes)

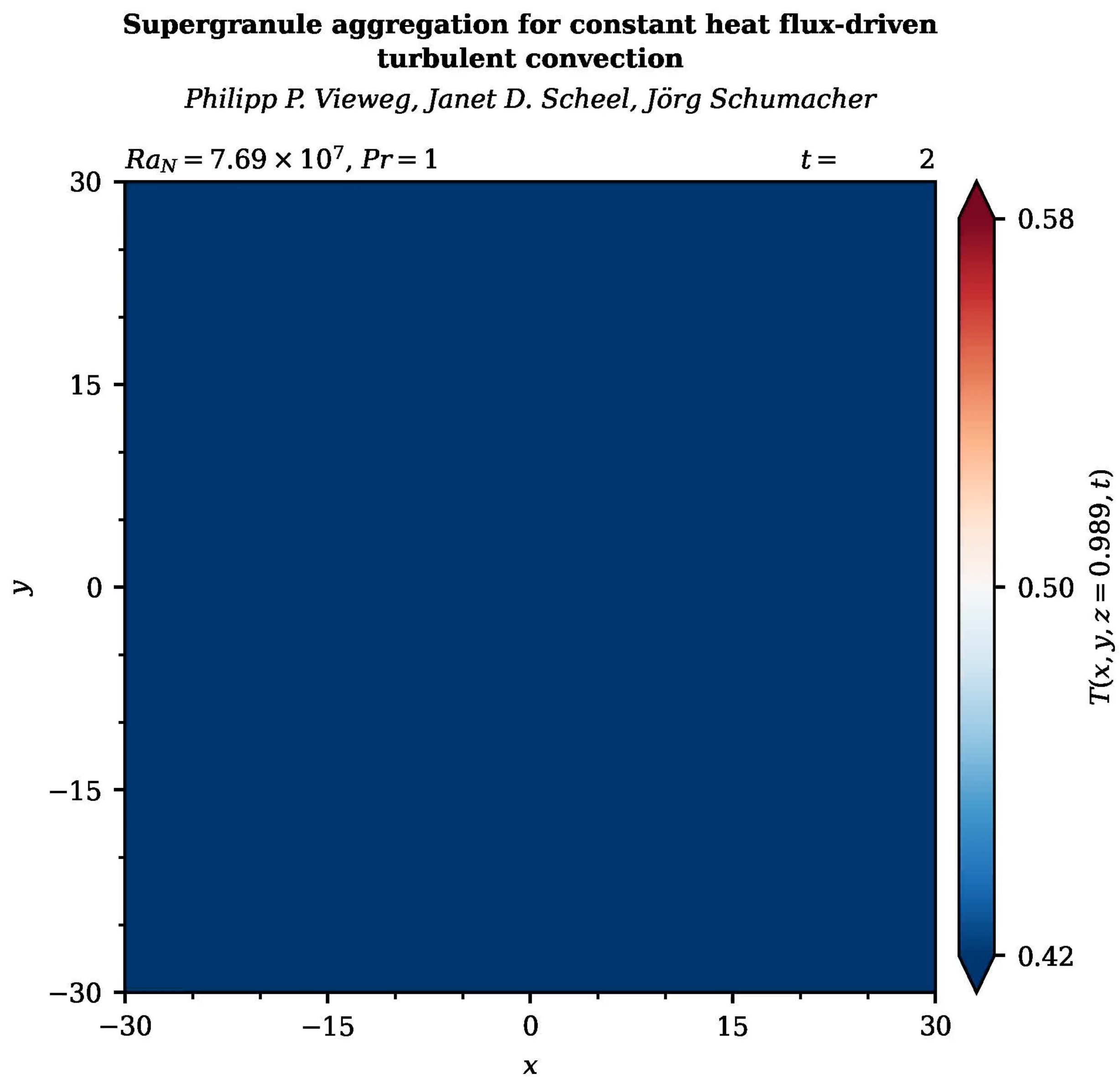
Comparison

$$T(x, y, z = 1 - \delta_T/2, t_0)$$



Temperature boundary conditions matter!

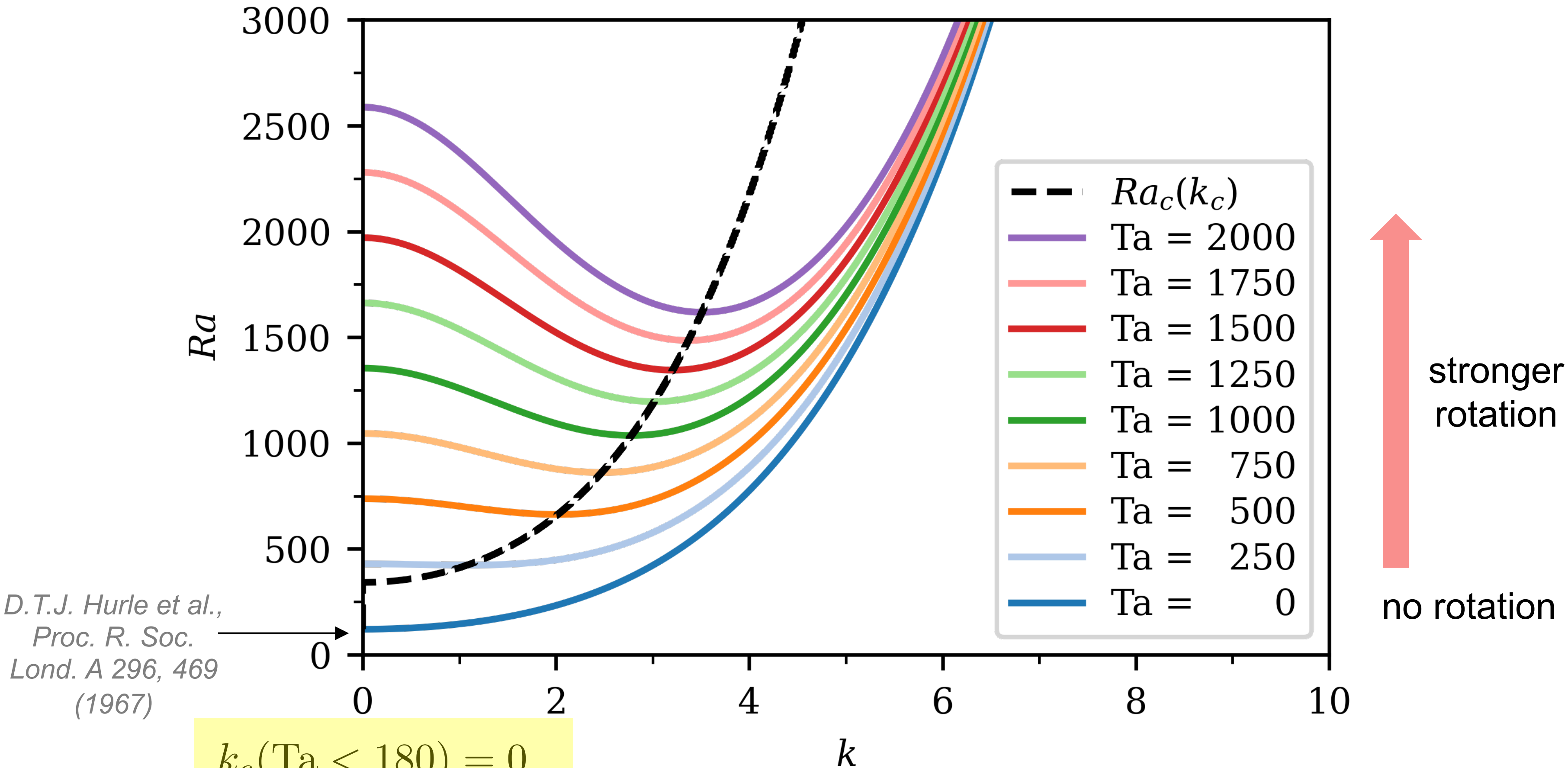
Long-term slow aggregation



What follows from linear stability theory?

T.E. Dowling, Woods Hole Summer Program 1988, Report No. WHOI-89-26

$$\mathrm{Ro} = \frac{\sqrt{g\alpha\Delta T}}{2\Omega\sqrt{H}} \longleftrightarrow \mathrm{Ta} = \frac{\mathrm{Ra}}{\mathrm{Ro}^2\mathrm{Pr}}$$



$k_c(\mathrm{Ta} < 180) = 0$

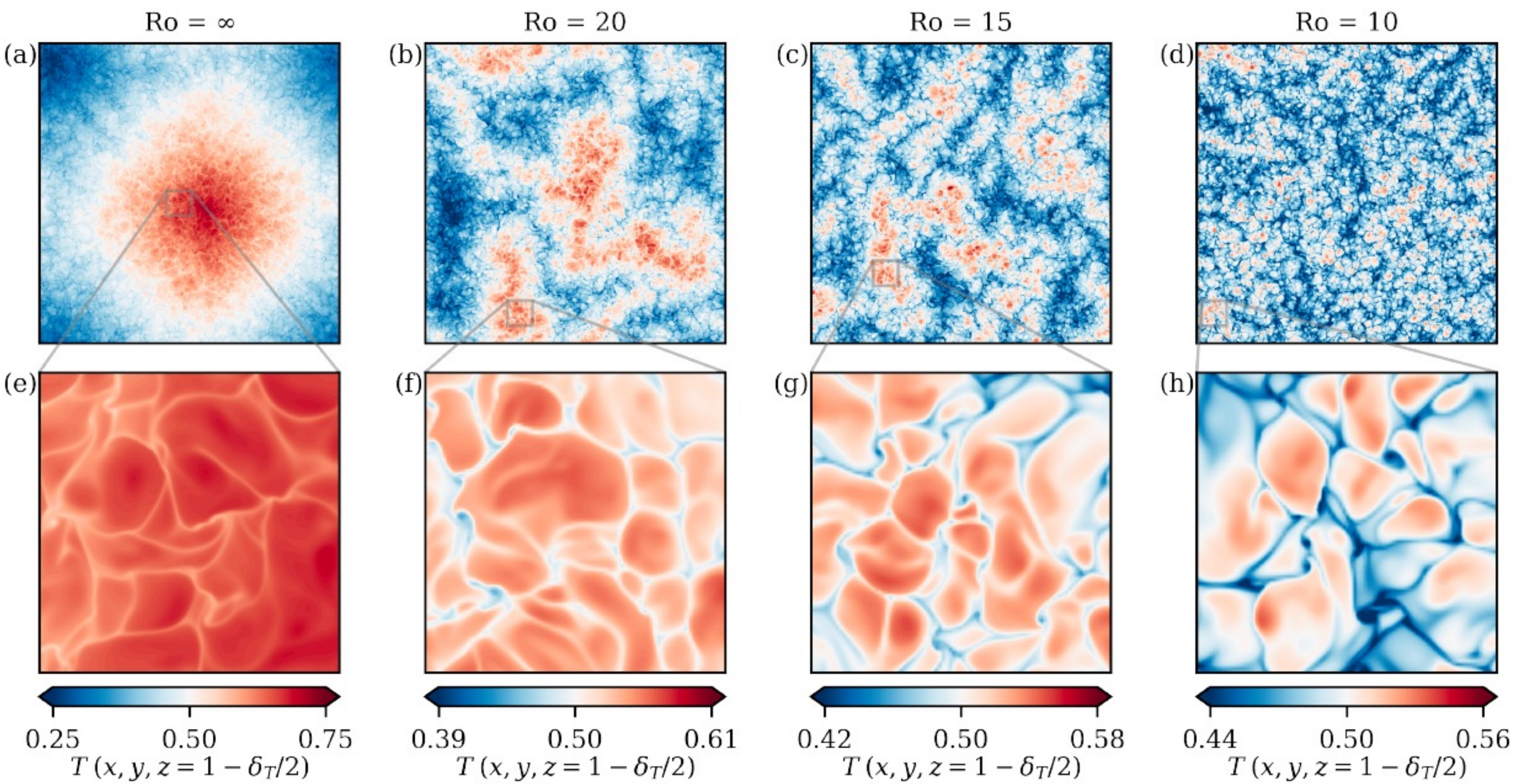
Critical wavenumber > 0 for sufficiently strong rotation

Strong and weak rotation

weakest rotation

$$Ra_N = 3.93 \times 10^6$$

strongest rotation



Increasing rotation rate reduces characteristic pattern scale

*G.M. Vasil, K. Julien, and N. Featherstone, PNAS **118**, e2022518118 (2021)*

- Role of boundary conditions
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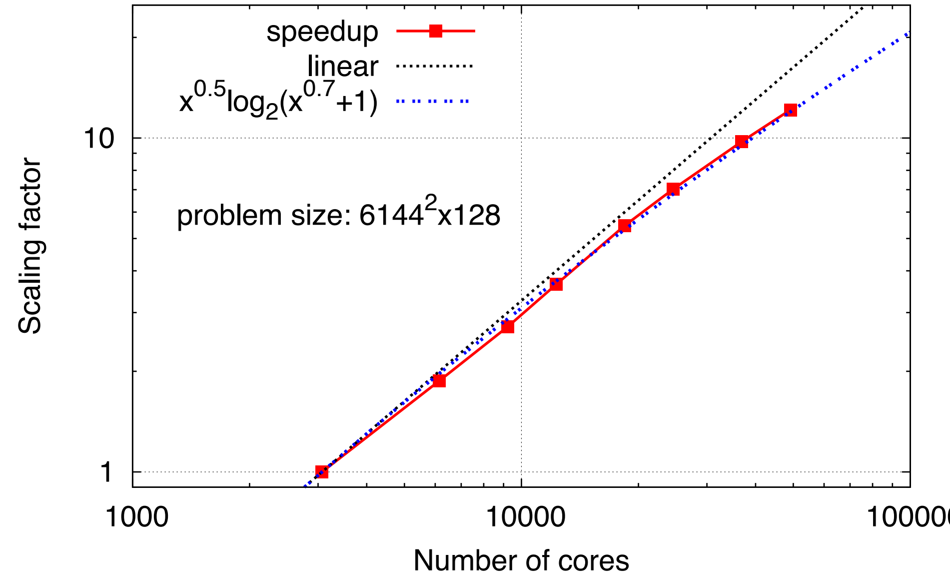
D. Krasnov

A. Pandey

DNS on SuperMUC-NG

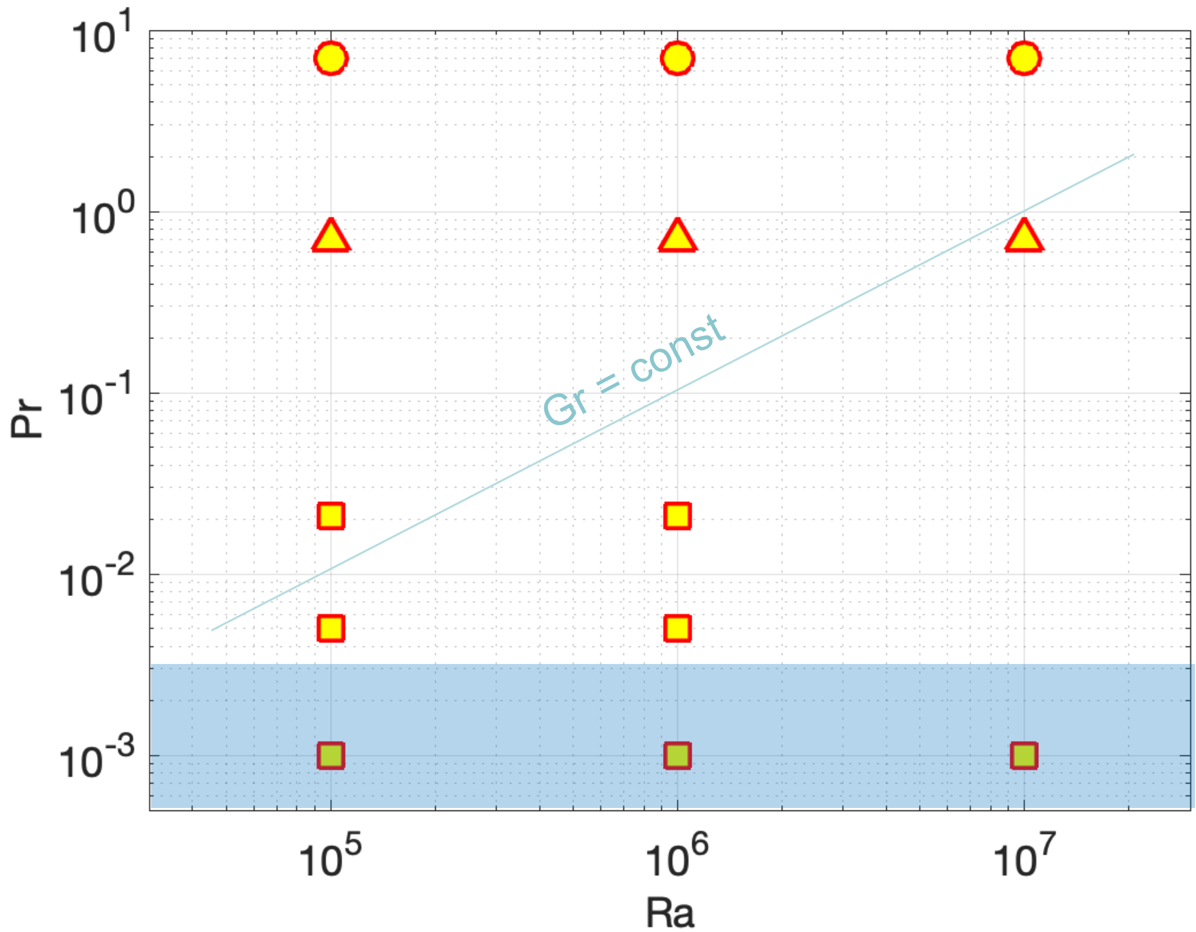


Biggest low-Pr DNS at LRZ Garching

- 5.37×10^{11} grid points for domain 25:25:1
- 144000 cores = 6000 MPI tasks × 24 OpenMP threads
- 3000 thin nodes with 48 cores/node with 90 GB per node
- Wall time/step $3.83\times10^{-3}\ h$
- Time for Poisson solvers per step : 56%
- Parallelization degree: 90%
- One convective free-fall time unit ≈ 30 million core-h
- One data snapshot (u_i, T) ≈ 17 TByte

Series of three-dimensional DNS

All at aspect ratio = 25



Water

TECHNISCHE UNIVERSITÄT ILMENAU

Air

Binary gas mixtures

GaInSn

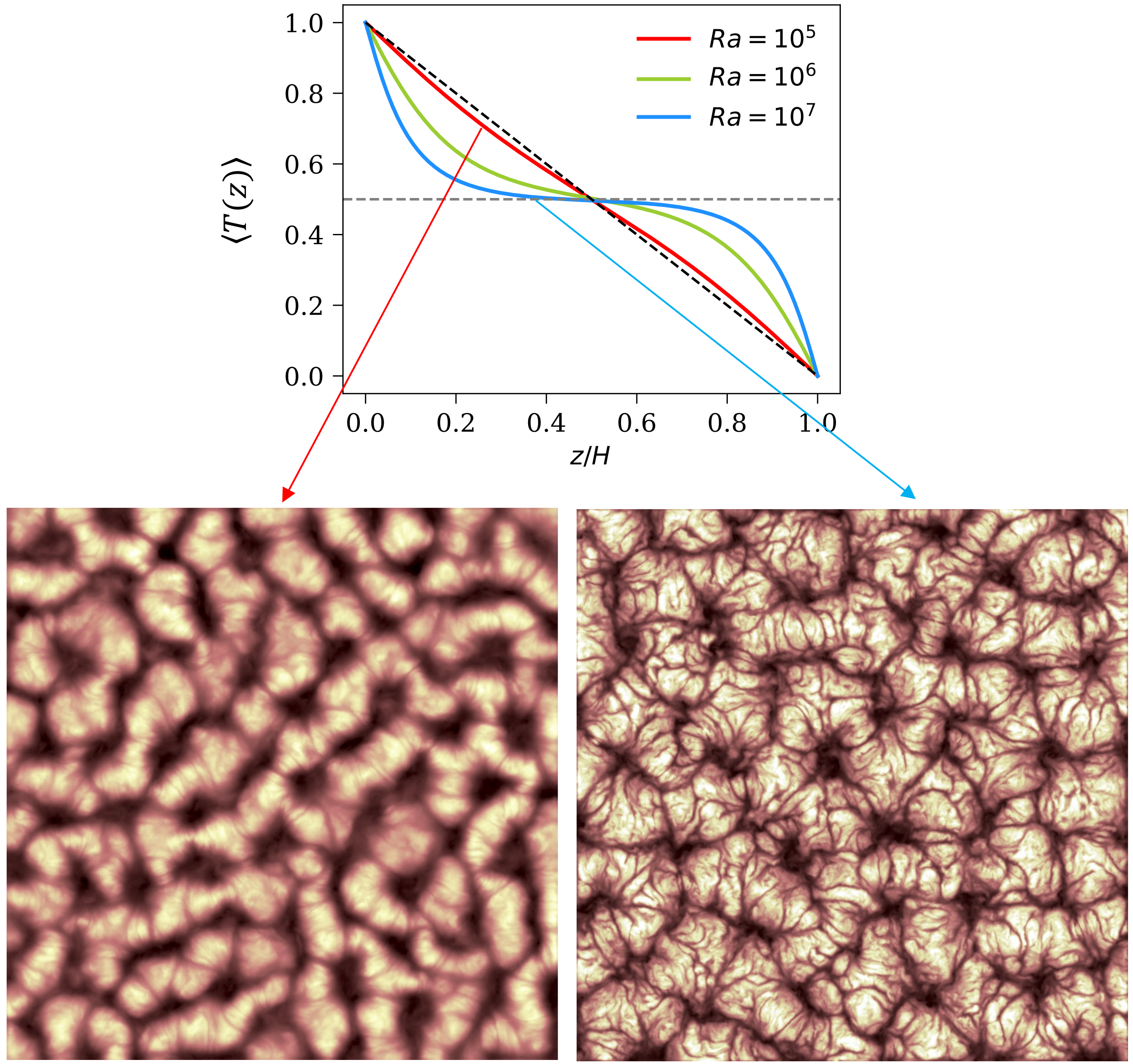
HZDR

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Sodium

No experiments possible!

Temperature fields at Pr=10^{-3}

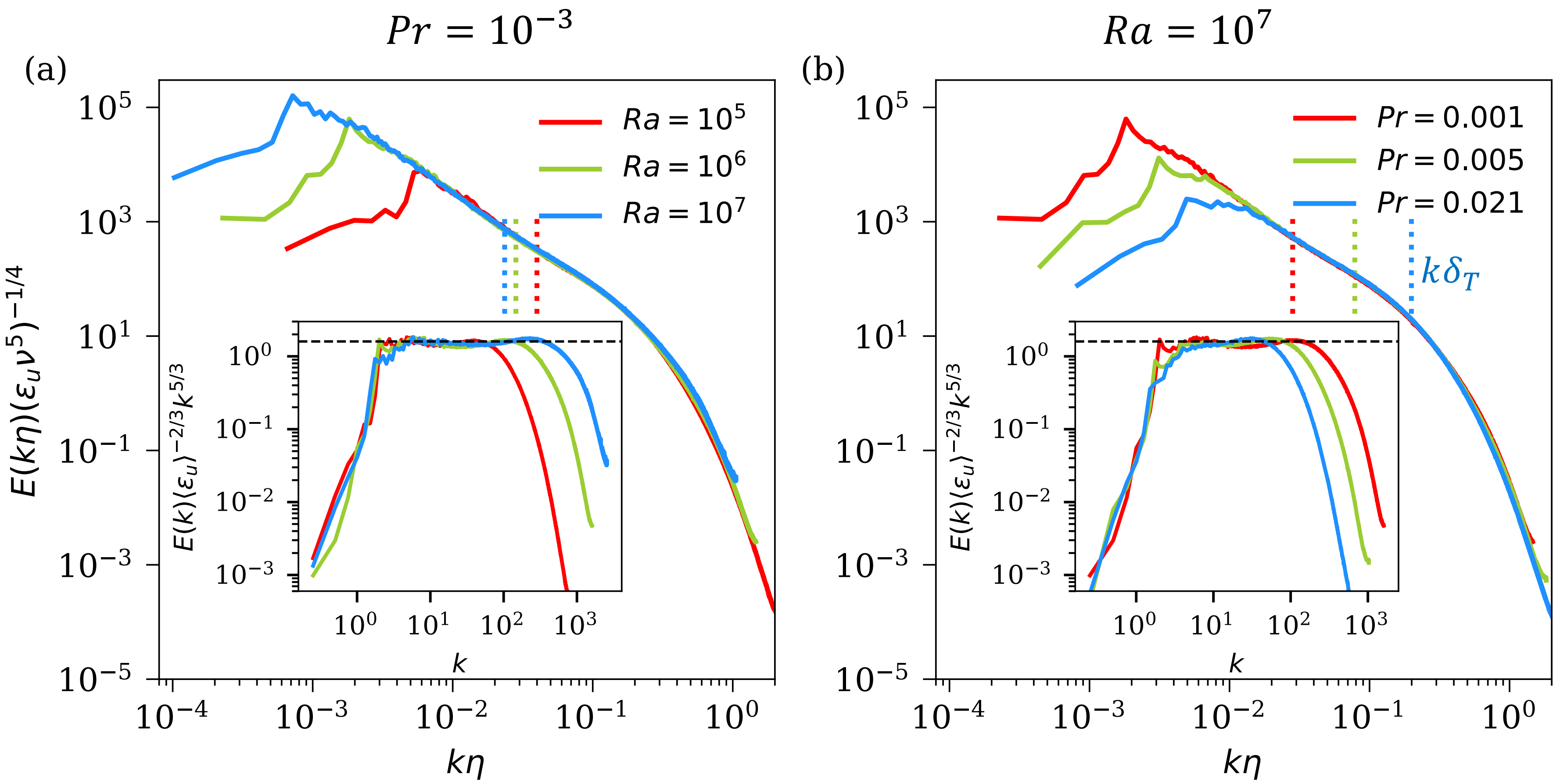


Ra=10^5

Ra=10^7

Is the bulk turbulence Kolmogorov-like?

$$E(k) = C_k \langle \varepsilon \rangle^{2/3} k^{-5/3}$$



Kolmogorov constant $C_k \approx 1.6$ agrees with the one in homogeneous isotropic turbulence

Alexander von Humboldt
Stiftung / Foundation

NIC

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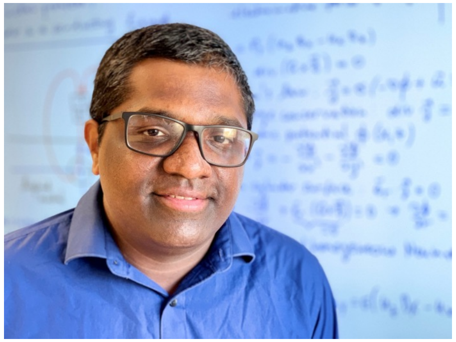


J. Panickacheril John

Compressible convection

J. Verhoeven et al., Astrophys. J. **805**, 62 (2015), C. Jones et al., J. Fluid Mech. **930**, A13 (2022)

Mass balance
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0\,,$$

Momentum balance
$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla p + \nabla \cdot \hat{\boldsymbol{\sigma}} - \rho g \boldsymbol{e}_z\,,$$

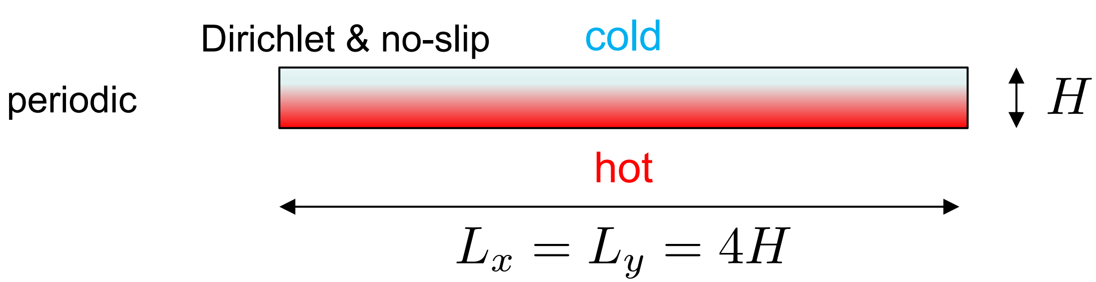
Energy balance
$$\frac{\partial (\rho e)}{\partial t} + \nabla \cdot (\rho e \boldsymbol{u}) + p \nabla \cdot \boldsymbol{u} = \nabla \cdot (k \nabla T) + \hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{S}}\,,$$

Equation of state
$$p = R \rho T \quad \text{with} \quad R = c_p - c_v\,,$$

Stress tensor
$$\hat{\boldsymbol{\sigma}} = 2 \eta \hat{\boldsymbol{S}} - \frac{2}{3} \eta (\nabla \cdot \boldsymbol{u}) \hat{\boldsymbol{I}}\,,$$

Internal energy density
$$\rho e = \rho c_v T\,, \quad T = \bar{T}(z) + T_{\mathrm{sa}}$$

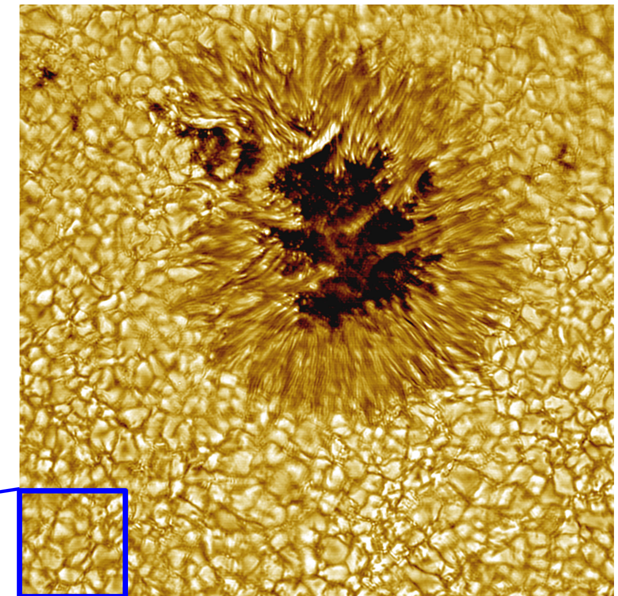
No bulk viscosity



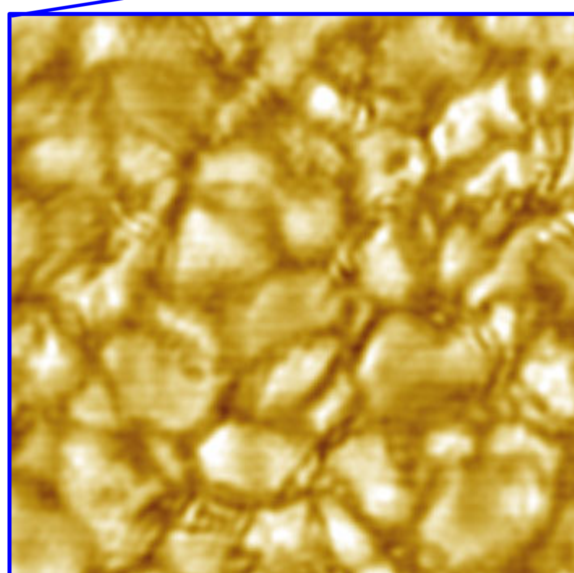
Why compressible?

JS and K.R. Sreenivasan, Rev. Mod. Phys. **92**, 041001 (2020)

- Strongly stratified mean profiles of p, ϱ, T
- Scale heights smaller than layer height
- Highly asymmetric convection patterns
- T-dependent material parameters
- Boundary layer growth affected by compressibility
- Characteristic sinking velocities $\sim c_s$



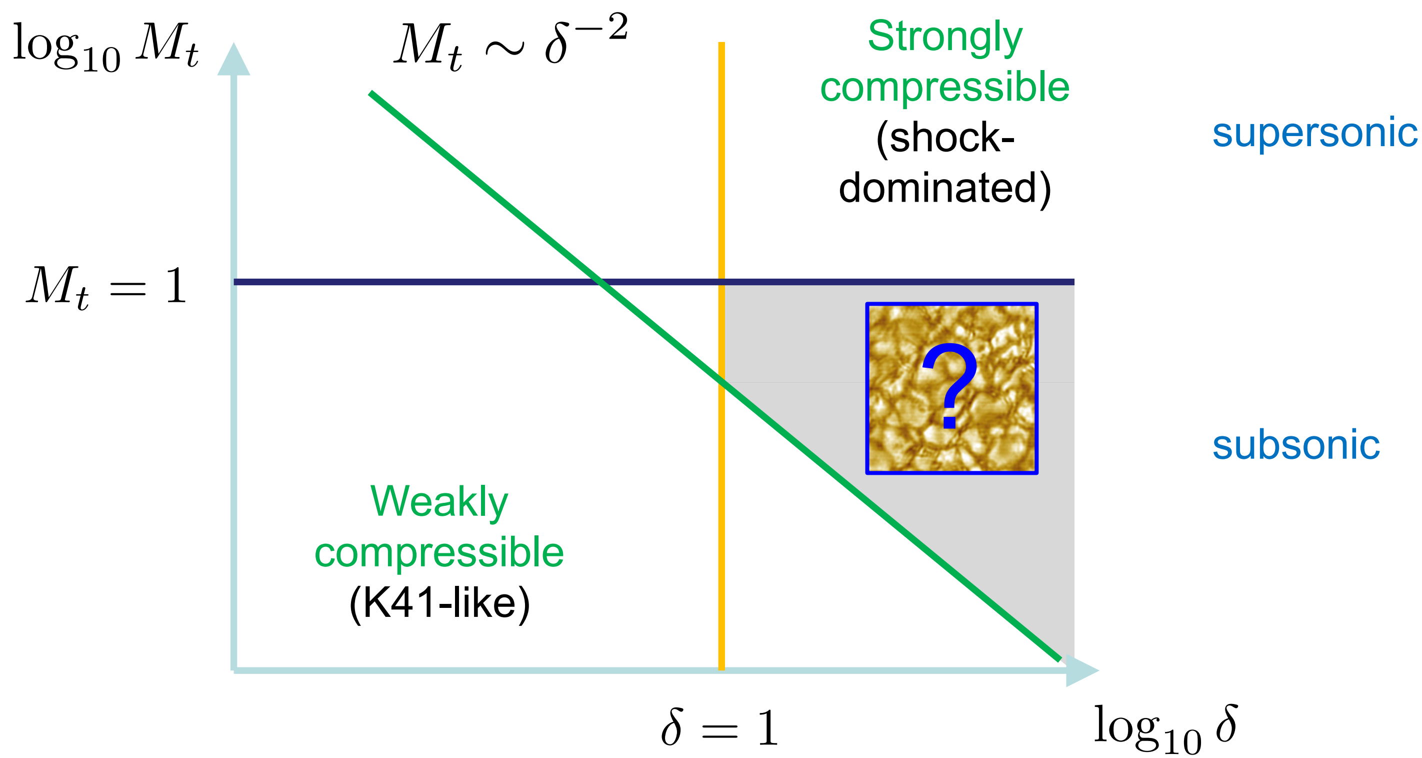
nasa.gov



Regimes of compressible turbulence

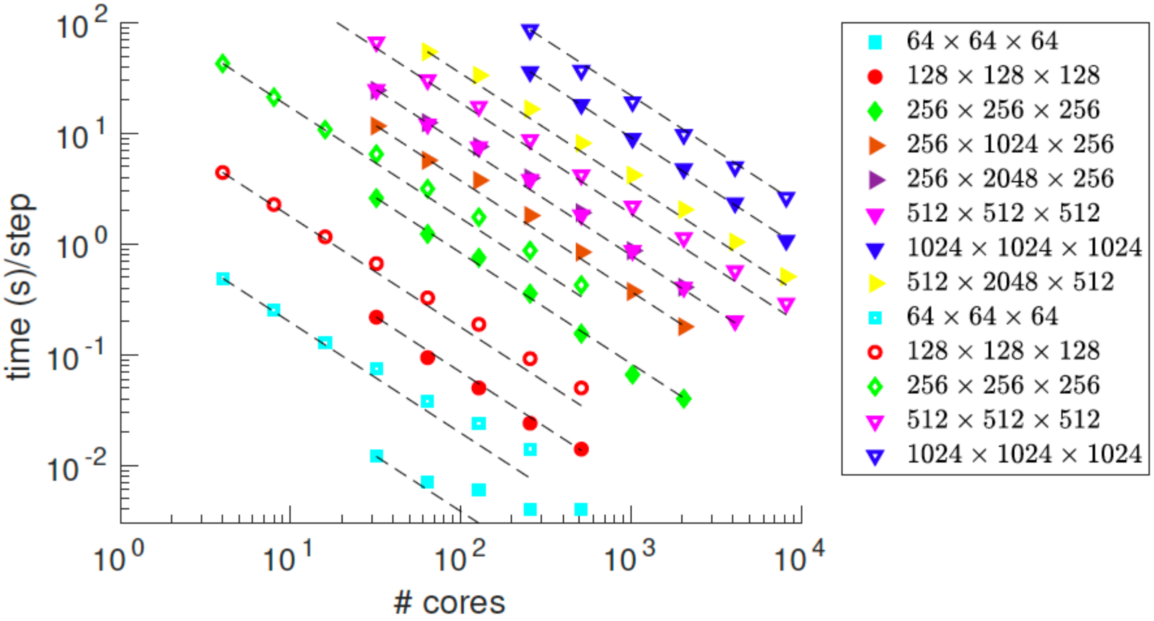
*J. Panickacheril John and D. A. Donzis, Phys. Rev. Fluids **5**, 084609 (2020)*

$$M_t = \frac{u'}{c_s} \qquad \delta = \frac{u'_d}{u'_s}$$



Helmholtz decomposition: $u_i = u_{i,s} + u_{i,d}$

DNS on Juwels Booster



- 6th- or 10th-order compact finite difference scheme using Padé approximation

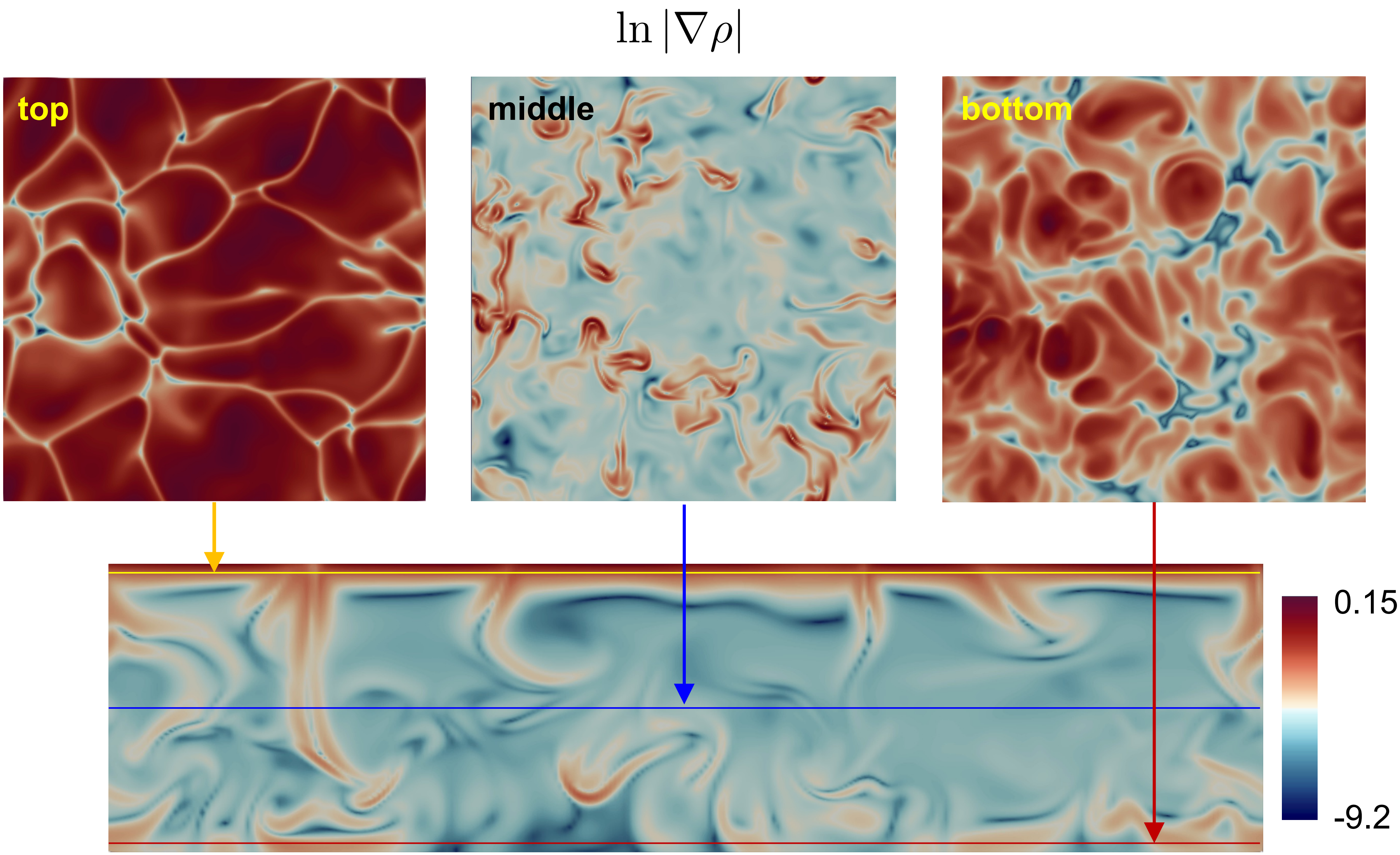
- Pure MPI code and Hybrid CPU/GPU
- 3d domain decomposition into pencils
- Forcing ρf_i in NS equation (most expensive) via OpenACC on GPUs
- Reduction of CPU time/step by 50%

Isotropic Compressible Turbulence

- Portation of the whole code on GPUs will require different domain decomposition

Compressible Convection

Density gradient at Ra=10^6 and Pr=0.7

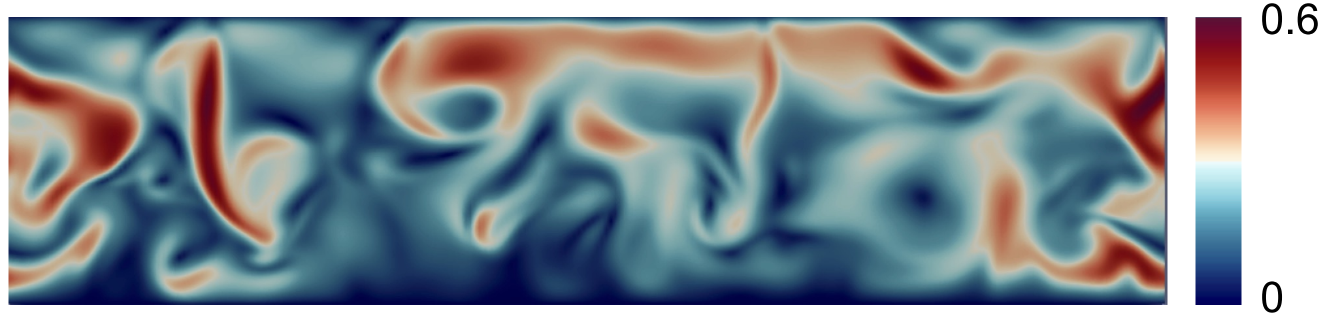


Highly asymmetric boundary layers!

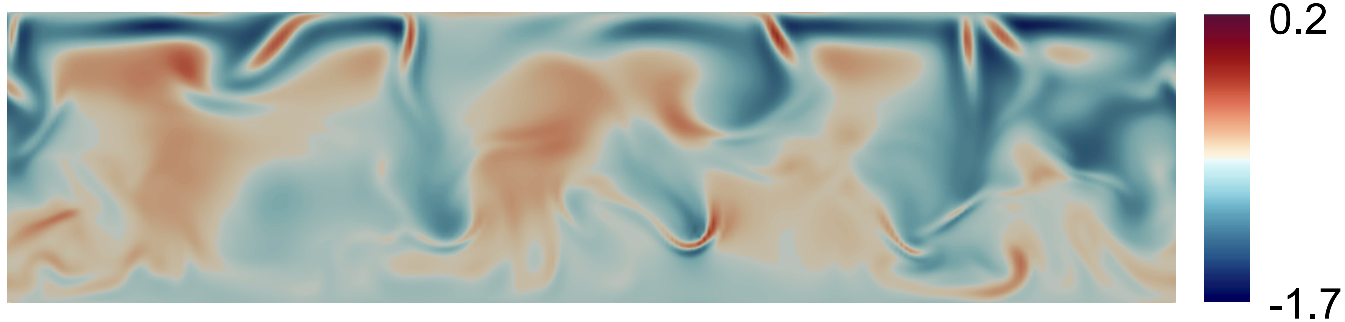
Features of compressibility

Three different measures to quantify the compressibility effects in turbulent convection

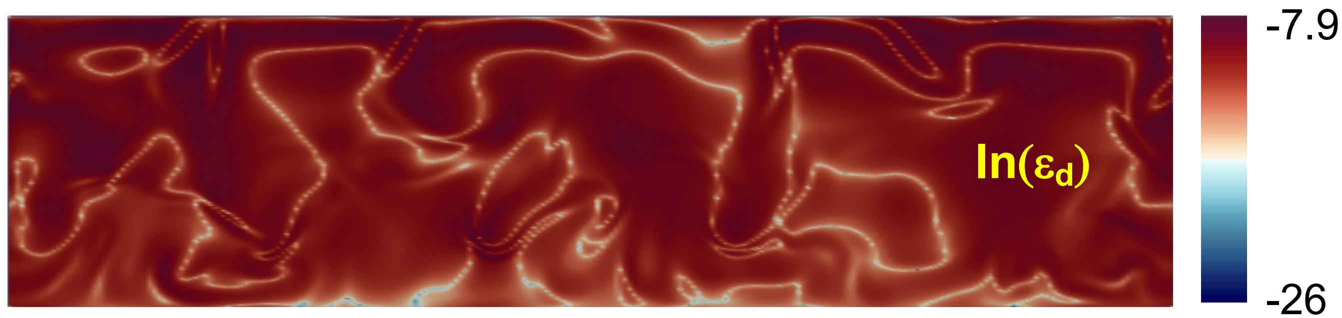
$$M_t = \frac{u'}{c_s}$$



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



$$\epsilon = \frac{\rho\nu}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)^2 + \frac{4\rho\nu}{3}(\nabla \cdot \mathbf{u})^2$$



Impact on small-scale intermittency and bulk mixing

Carl Zeiss Stiftung

NIC

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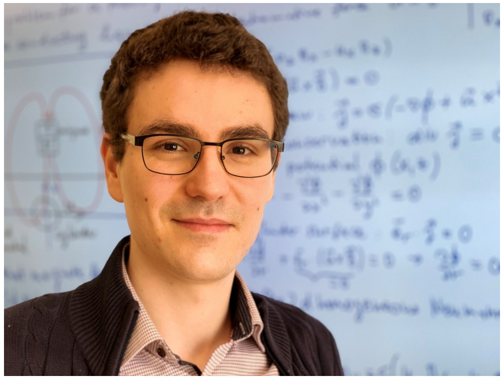
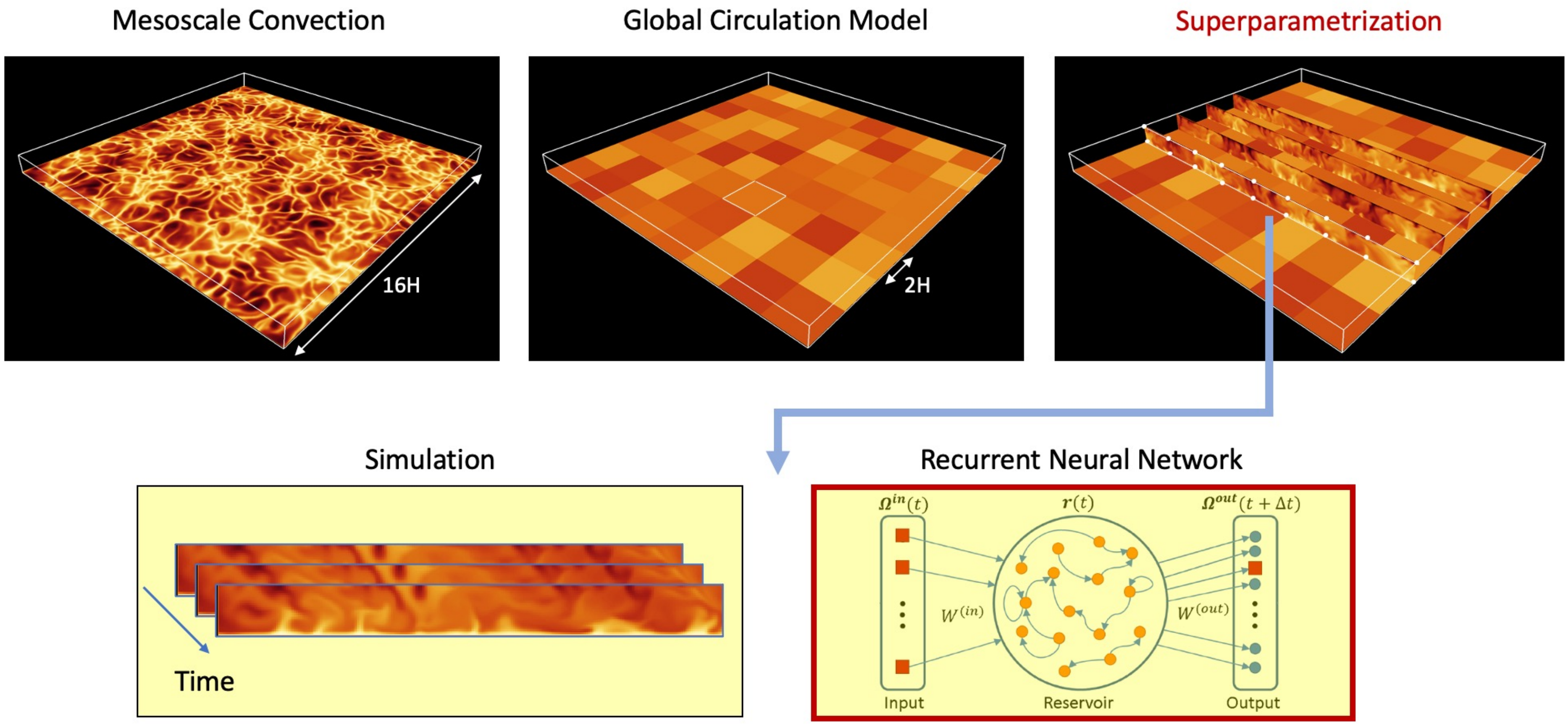


F. Heyder

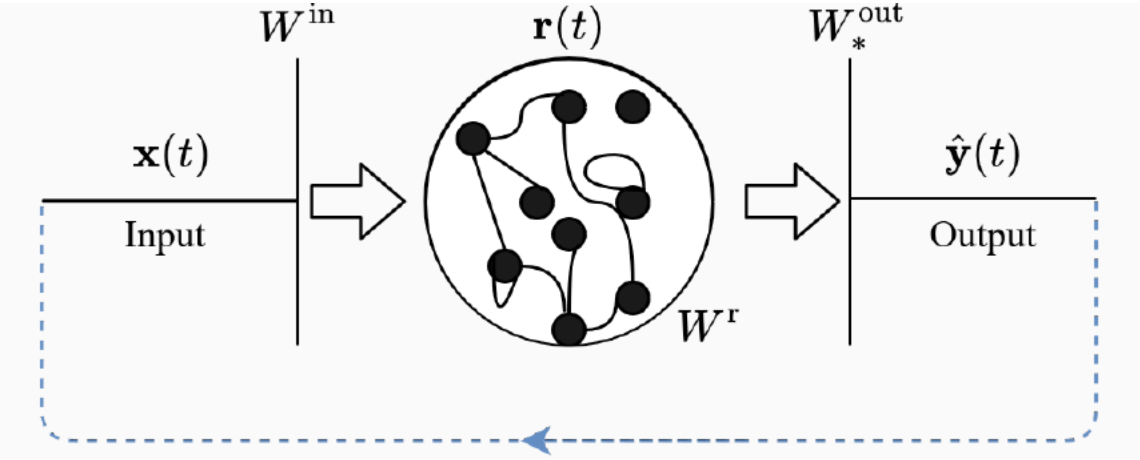
P. Pfeffer

Superparametrization



- Generalization properties of the neural network
- Fast and cheap neural network implementation
- Scalable model to realistic dimensionless parameters

Reservoir computing model



H. Jaeger, GMD report 148 (2001)

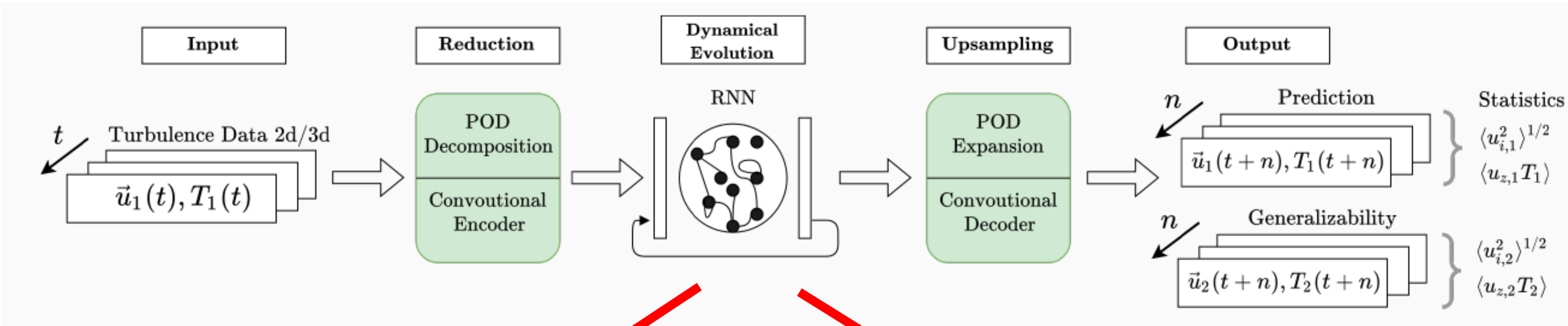
- Reservoir = Sparse random network initially initialized (density 20%)
- Input matrix also random
- Reservoir dynamics

$$\mathbf{r}_t = (1-\alpha)\mathbf{r}_{t-1} + \alpha \tanh(W^{in}\mathbf{x}_t + W^r\mathbf{r}_{t-1})$$

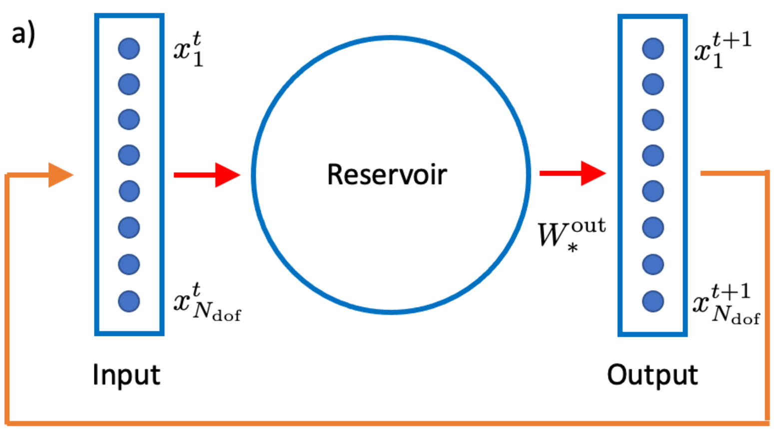
memory nonlinear activation

- Output layer is trained only $\hat{\mathbf{y}}_t = W_*^{out}\mathbf{r}_t \approx \mathbf{x}_{t+1}$
- Hyperparameters: Number of reservoir nodes
  Reservoir node density
  Spectral radius of reservoir
  Leaking rate α
  Ridge regression parameter in loss

Machine learning pipeline

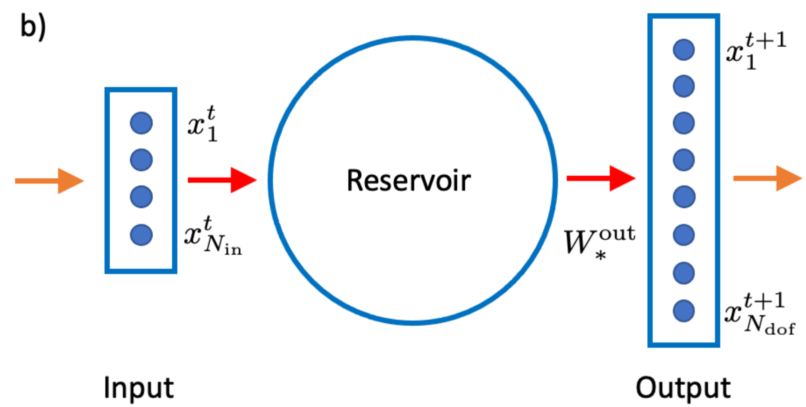


Closed loop mode reservoir computing model



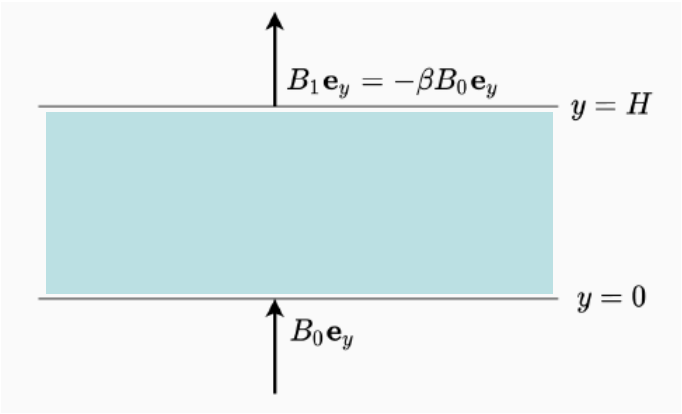
Autonomously operating recurrent network for prediction

Open loop mode reservoir computing model



Recurrent network for reconstruction

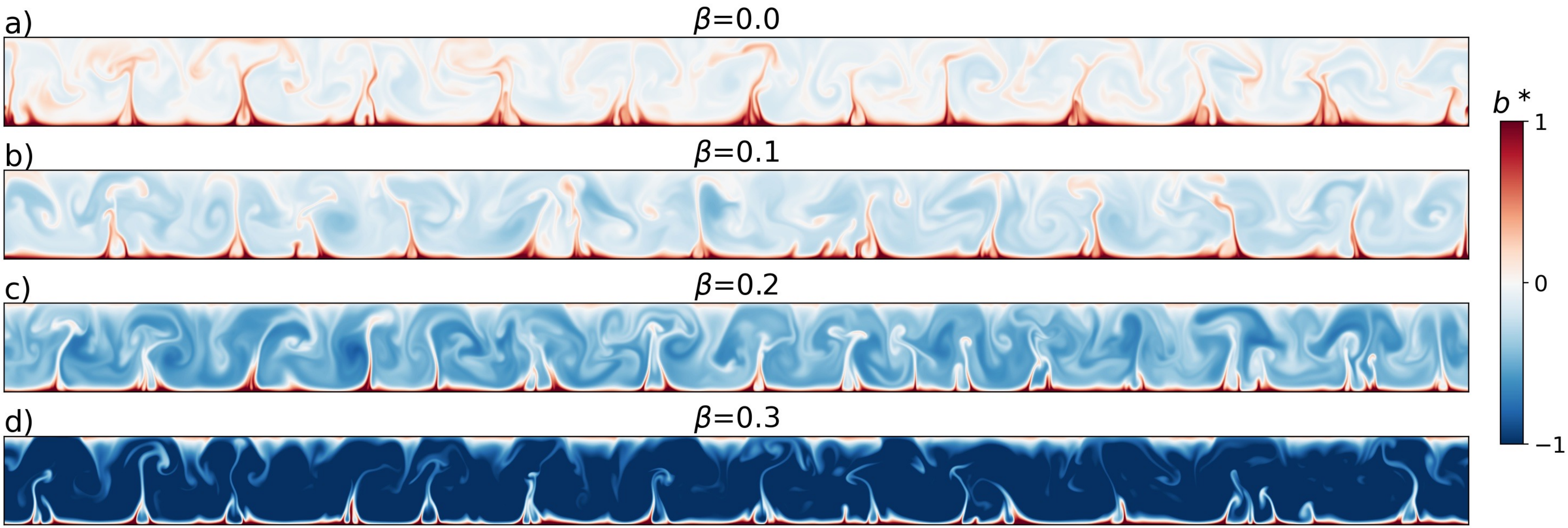
Closed loop mode



2d model of a convective boundary layer

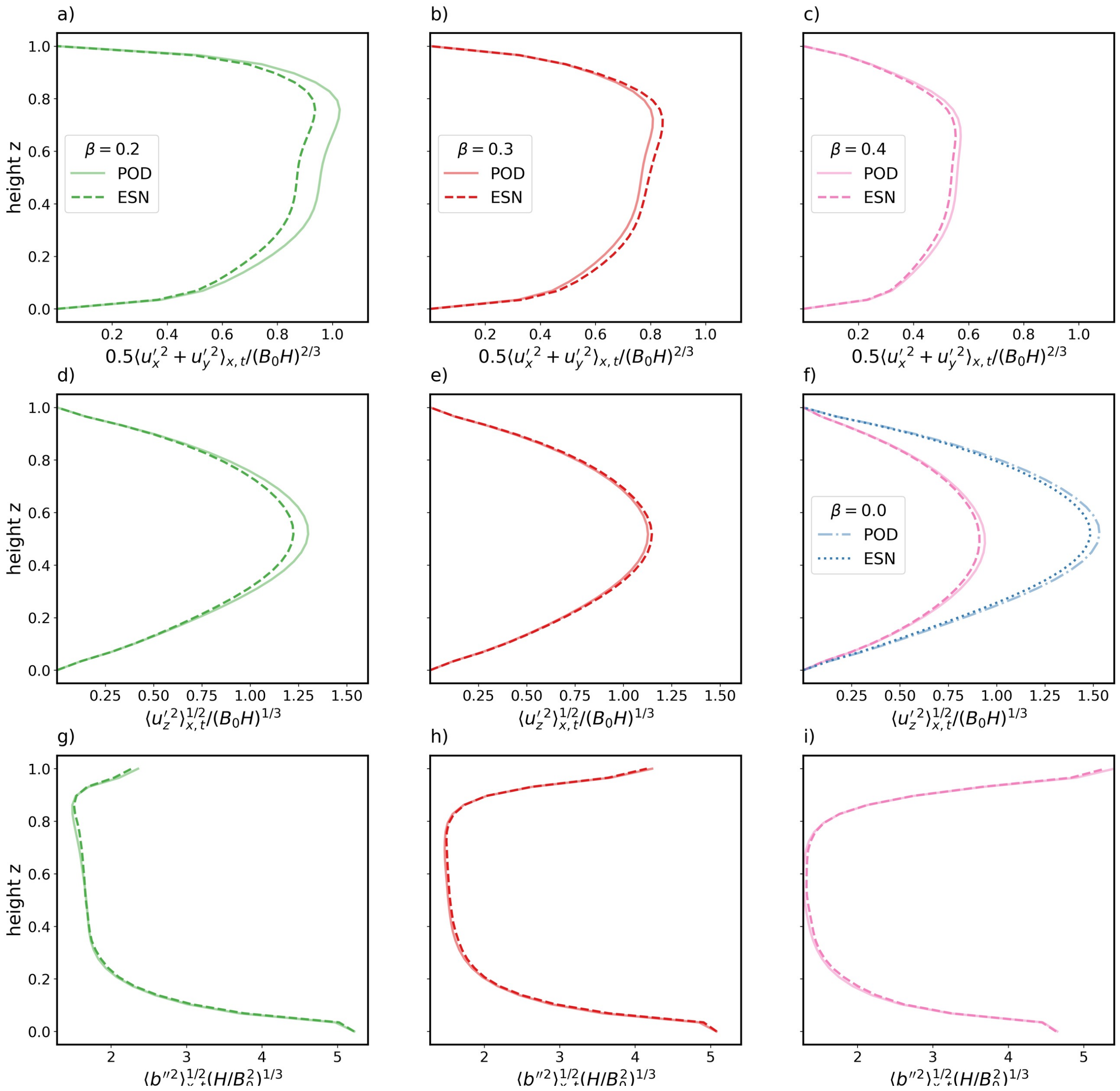
Heat-flux-driven from bottom and top

Closed loop mode
Data reduction with POD/CAE



Train for $\beta = 0.1$ and predict for unseen $\beta = 0.2, 0.3$

Predicted profiles

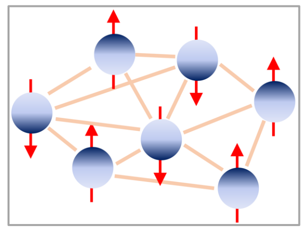


Quantum Reservoir Computing

*D. Markovic and J. Grollier, Appl. Phys. Lett. **117**, 150501 (2020)*

QRC

Analog QRC



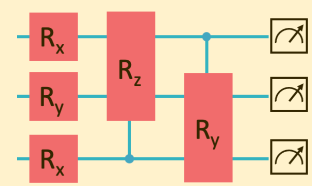
Unitary time evolution

$$|\Psi(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\Psi_0\rangle$$

with

$$\hat{H} = -\sum_{i<j} J_{ij}\hat{Z}_i\hat{Z}_j - \sum_i h_i\hat{Z}_i$$

Digital QRC



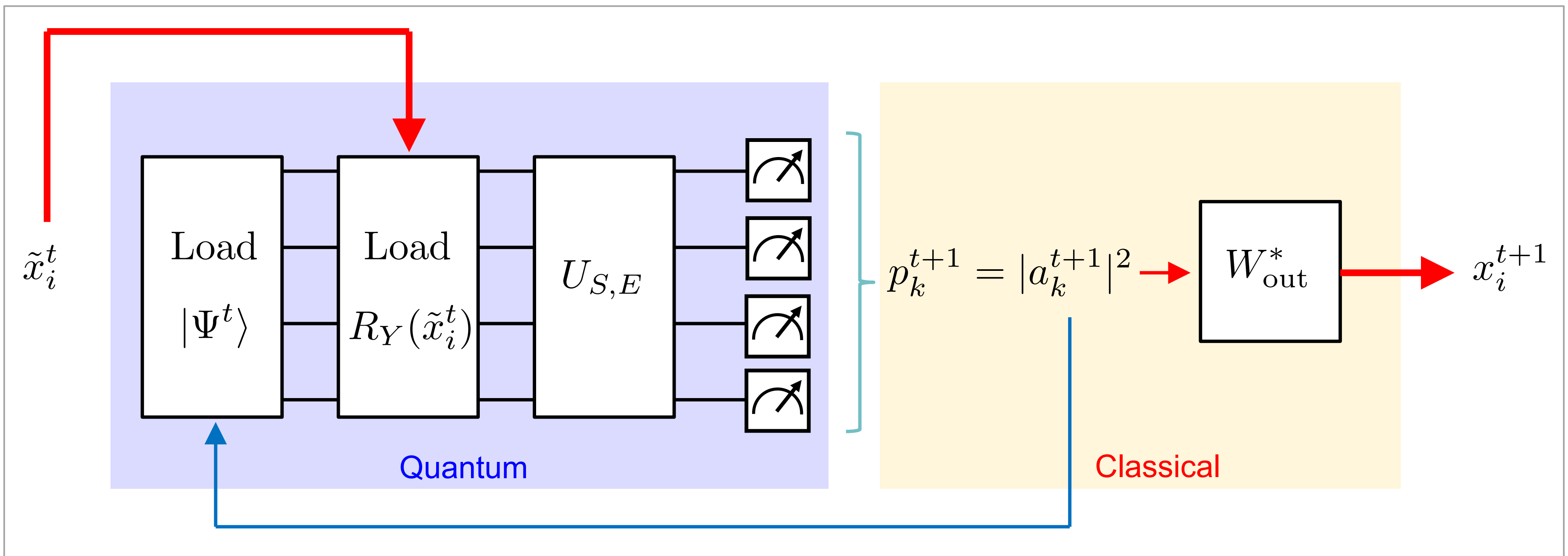
Unitary transformation

$$|\Psi(t)\rangle = \prod_{j=1}^{d}\left(\hat{R}_i(\theta_j)\hat{U}_E\right)|\Psi_0\rangle$$

Substitute the classical sparse reservoir network by a highly entangled n-qubit quantum state

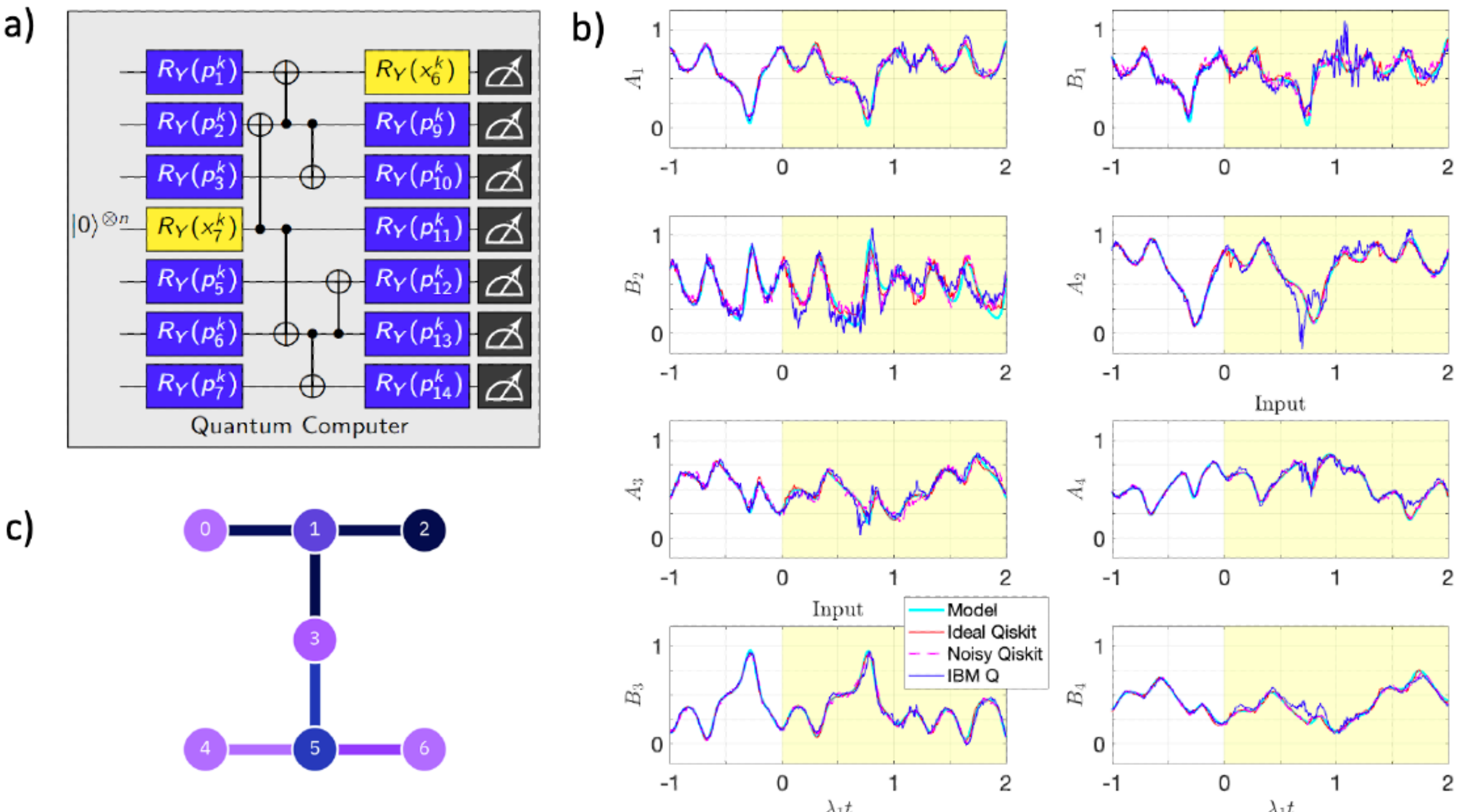
Hybrid quantum-classical open loop mode

- Dynamical system $x_i^{t+1} = f_i(x_j^t, \alpha_1, \ldots, \alpha_K) \quad i, j = 1, \ldots, M$
- Number of qubits n
- Quantum reservoir state $|\Psi^t\rangle = \sum_{k=0}^{2^n-1} a_k^t |k\rangle$
- Partial continued input $\tilde{x}_1^t, \ldots, \tilde{x}_K^t \quad K \ll M$



Implementation on IBM-Q

8-dimensional Lorenz-type model of a Rayleigh-Bénard flow



7 superconducting qubits

Proof of concept for strongly reduced quantum reservoir

Quantum Advantage?

PRX QUANTUM **3**, 030101 (2022)

Perspective

Is Quantum Advantage the Right Goal for Quantum Machine Learning?

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(Received 18 November 2021; revised 16 May 2022; published 14 July 2022)

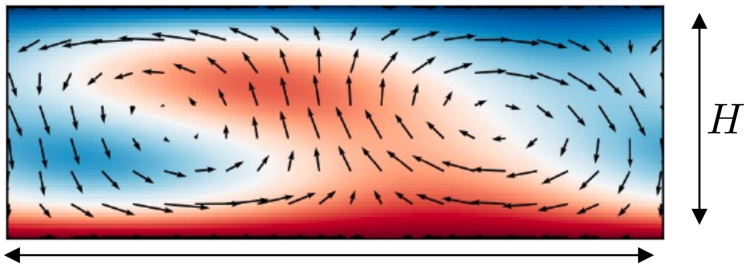
	Classical RCM	Quantum RCM
Reservoir dimension	$N^c_{\text{res}} = N$	$N^q_{\text{res}} = 2^n$
Number of shots		$K = 2^{10+n}$
Operations with reservoir	$N^2 + N_{\text{in}} N \sim N^2$	$K \times \xi n$ $\quad \xi \sim \mathcal{O}(1)$

$$N > 2^{10} \xi \log_2 N \quad \text{if} \quad N^c_{\text{res}} = N^q_{\text{res}} = N = 2^n$$

Two points:
- Requires: $n \geq 16$ Typically $N^c_{\text{res}} \gg N^q_{\text{res}}$
- Load into the quantum register ($\xi = const$?)

What‘s next?

8D weakly nonlinear model

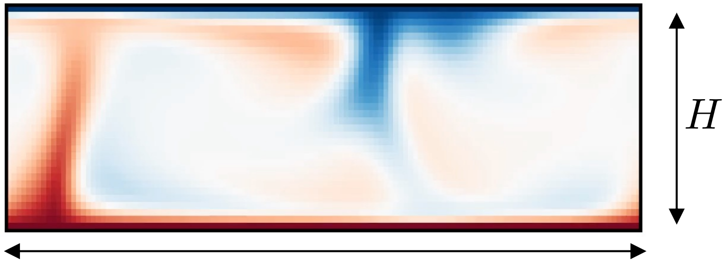


$L = 2\sqrt{2}H$

$Pr = 10$

$Ra = 1.8 \times 10^4$

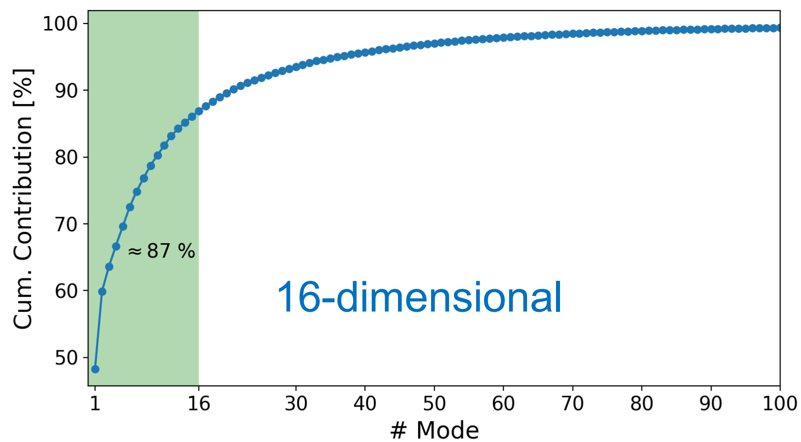
Turbulent model

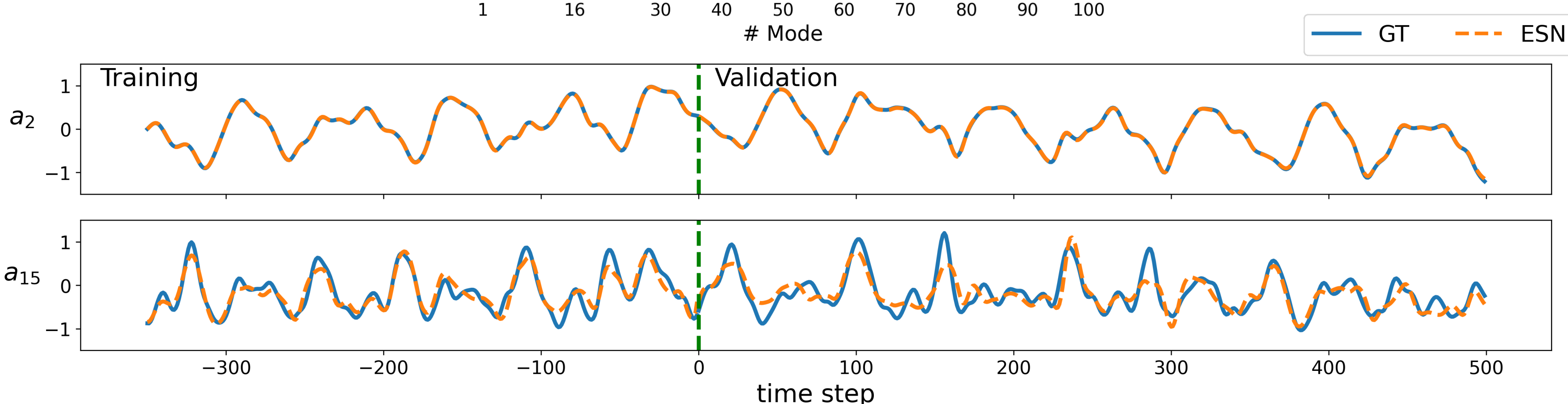


$L = 2\sqrt{2}H$

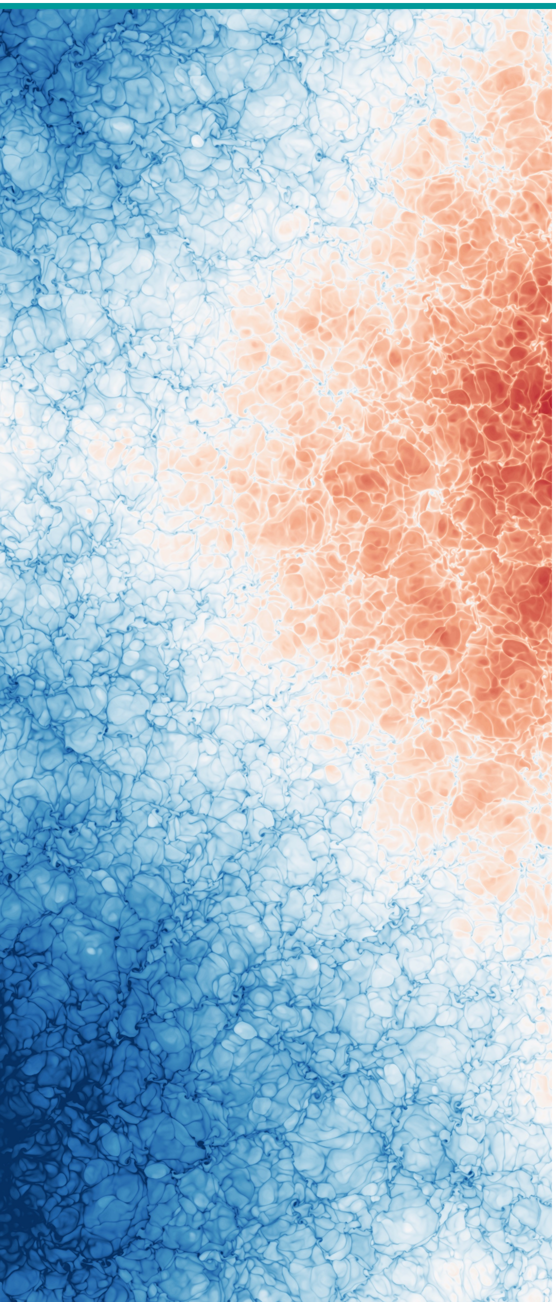
$Pr = 10$

$Ra = 10^5$





Summary



- Supergranule-granule hierarchy in simple RBC flow with imposed flux boundary conditions
- Inverse cascade of the subset of horizontal modes in 3d heat-flux-driven flow causes supergranulation
- Additional rotation controls the breakdown of the inverse cascade and size of supergranule
- Very low Prandtl number convection is Kolmogorov-like in the bulk
- Fully compressible convection results in asymmetric up- and downflows and boundary layers and enhanced intermittency by pre-shock regions
- Reduced dynamical model of turbulent convection by reservoir computing as a convective parametrization
- Proof-of-concept for hybrid quantum-classical reservoir computing model of convection flow

References

- Supergranule-granule hierarchy
  P.P. Vieweg, J.D. Scheel, JS, Phys. Rev. Research **3**, 013231 (2021)
  P.P. Vieweg, J.D. Scheel, R. Stepanov, JS, arXiv:2207.12606 (2022)

- Very low Prandtl numbers
  A. Pandey, JS, K.R. Sreenivasan, Astrophys. J. **907**, 56 (2021)
  A. Pandey, D. Krasnov, K.R. Sreenivasan, JS, J. Fluid Mech. **948**, A23 (2022)
  A. Pandey, D. Krasnov, JS, R. Samtaney, K.R. Sreenivasan, Physica D, in press (2022)

- Machine learning in turbulent convection
  F. Heyder, JS, Phys. Rev. E **103**, 053107 (2021)
  S. Pandey, P. Teutsch, P. Mäder, JS, Phys. Fluids **34**, 045106 (2022)
  F. Heyder, J.P. Mellado, JS, Phys. Rev. E, in press (2022)

- Quantum algorithms of classical dynamical systems
  D. Giannakis, A. Ourmazd, P. Pfeffer, JS, J. Slawinska, Phys. Rev. A **105**, 052404 (2022)
  P. Pfeffer, F. Heyder, JS, Phys. Rev. Research **4**, 052404 (2022)

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Thanks!