Sustainability challenges in the water-energy-climate nexus
The role of computational science

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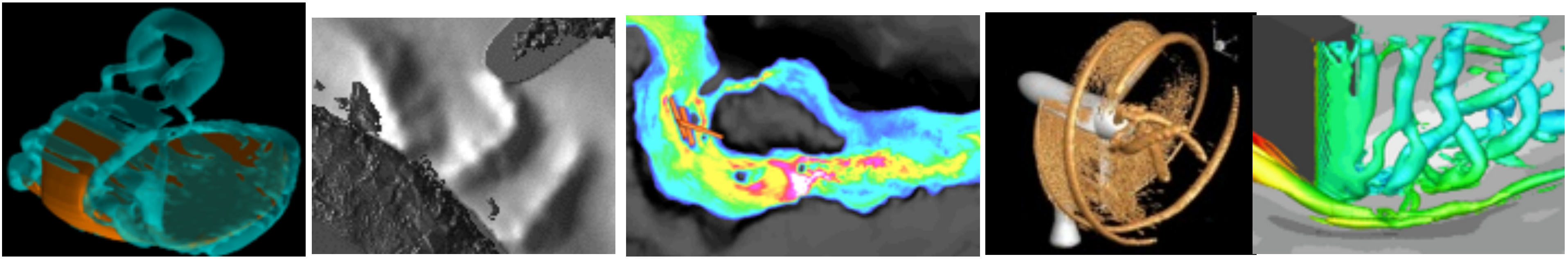
Stony Brook, NY



Tiscornia Lecture, University of Genova
Genova, September 30, 2016

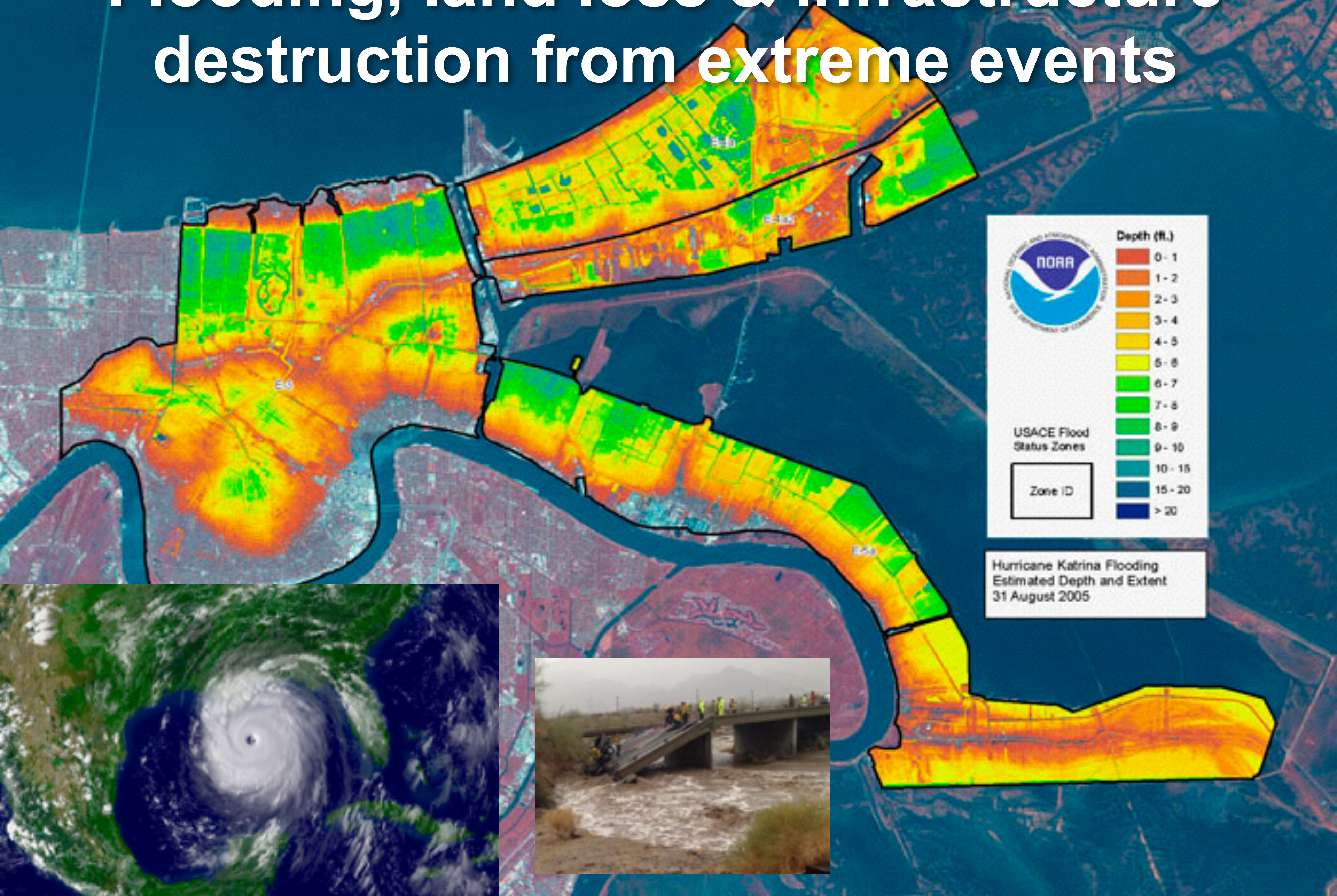
Anthropogenically-induced waterway degradation & biodiversity decline


Stream bank erosion


Excessive sediment loads


Algal blooms

Flooding, land loss & infrastructure destruction from extreme events



Marine & Hydrokinetic Technologies
The Energy/Water Nexus

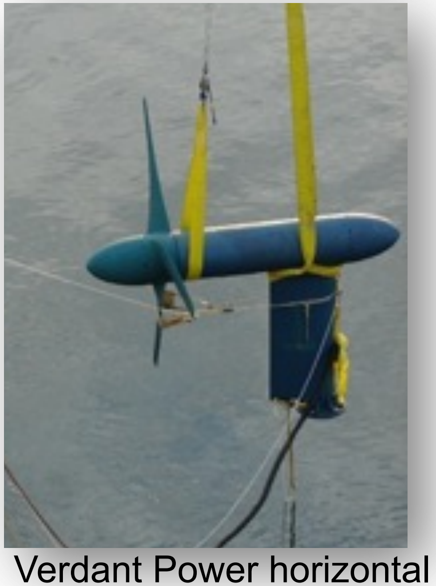
Ocean Power Technologies (OPT) wave point absorber

Hydro Green Energy river current turbine

OPD Pelamis wave generator

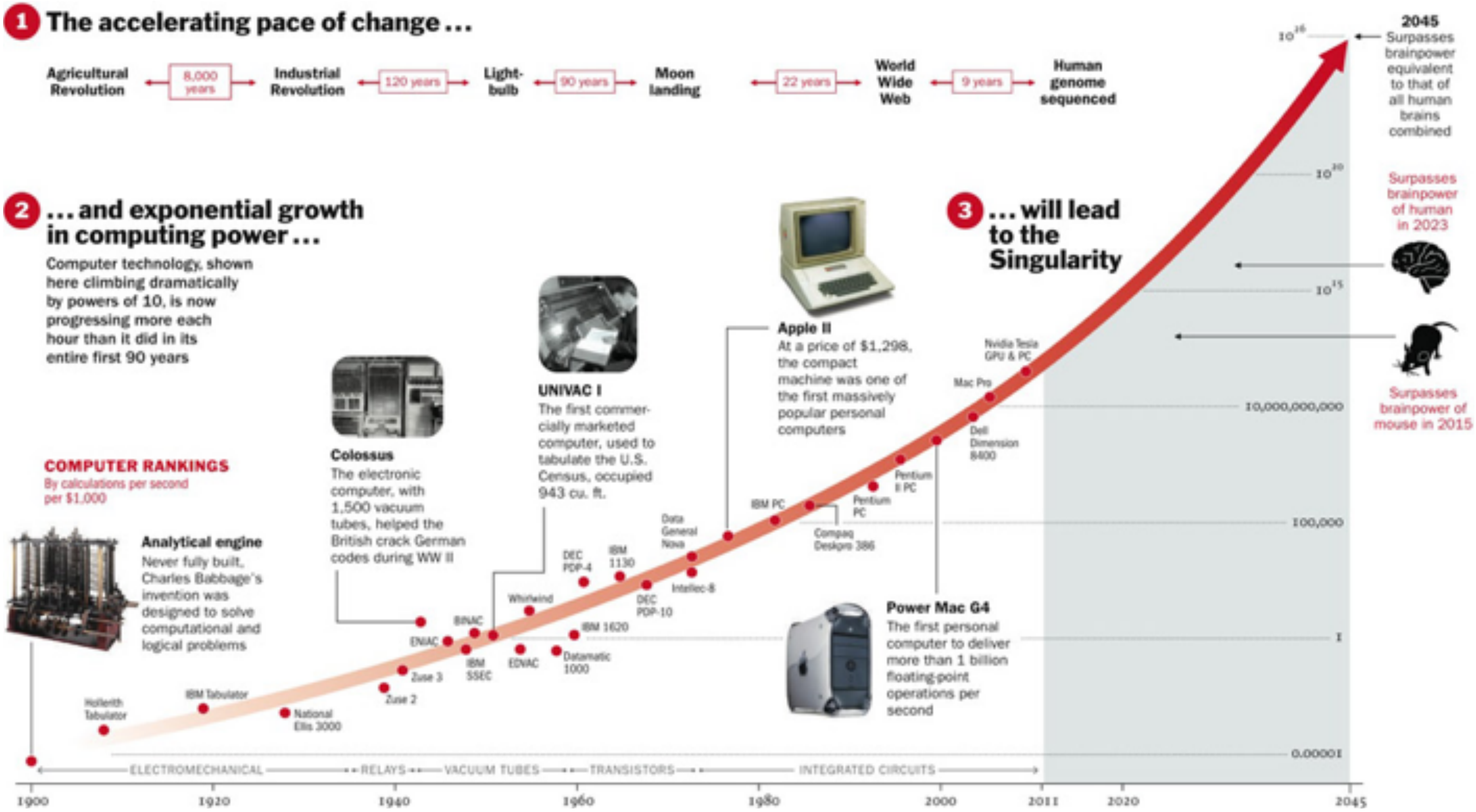
Vortex Hydro Energy VIVACE system

Marine Current Turbines tidal turbine



Verdant Power horizontal axial flow tidal turbine

Simulation-based engineering science leveraging exponential computing



1 The accelerating pace of change ...

2 ... and exponential growth in computing power ...

Computer technology, shown here climbing dramatically by powers of 10, is now progressing more each hour than it did in its entire first 90 years

3 ... will lead to the Singularity

COMPUTER RANKINGS

By calculations per second per $1,000

Analytical engine
Never fully built, Charles Babbage's invention was designed to solve computational and logical problems

Colossus
The electronic computer, with 1,500 vacuum tubes, helped the British crack German codes during WW II

UNIVAC I
The first commercially marketed computer, used to tabulate the U.S. Census, occupied 943 cu. ft.

Apple II
At a price of $1,298, the compact machine was one of the first massively popular personal computers

Power Mac G4
The first personal computer to deliver more than 1 billion floating-point operations per second

2045
Surpasses brainpower equivalent to that of all human brains combined

Surpasses brainpower of human in 2023

Surpasses brainpower of mouse in 2015

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Vision paper

Hydraulics in the era of exponentially growing computing power

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ABSTRACT
Recent advances in computational algorithms coupled with exponentially growing computing power pave the way for developing a powerful simulation-based engineering science framework for tackling a broad range of hydraulic engineering flows. Multi-physics simulations taking into account complex waterway bathymetry, energetic coherent structures, turbulence/sediment interactions and morphodynamics, free-surface effects and flow structure interaction phenomena are now well within reach and are beginning to impact engineering practice. I review such progress and offer specific examples highlighting the enormous potential of simulation-based engineering science to supplement and dramatically augment the insights that can be gained from physical experiments. I discuss major computational challenges that lie ahead but also underscore the enormous opportunities to take advantage of advanced algorithms, powerful supercomputers and big data to tackle societal challenges in restoration of aquatic environments, sustainable mitigation of the impacts of global environmental change, and development of efficient and environmentally compatible renewable energy systems.

Keywords: Complex hydraulic structures; data-driven models; energy–water nexus; flooding; large-eddy simulation; real-life waterways; sediment transport; simulation-based engineering science; turbulence

Data-driven cyber-physical systems approach

Riding the wave of high performance computing and exponential technologies

Data-driven simulations of turbulence in waterways

Big-data-driven HPC simulation of ecosystems: Hazard mitigation, water quality, energy harvesting, restoration & sustainability, etc.

Ecosystem scale: Data from satellites and airborne lidars

Local scale: Real-time data from embedded and autonomous robotic sensors

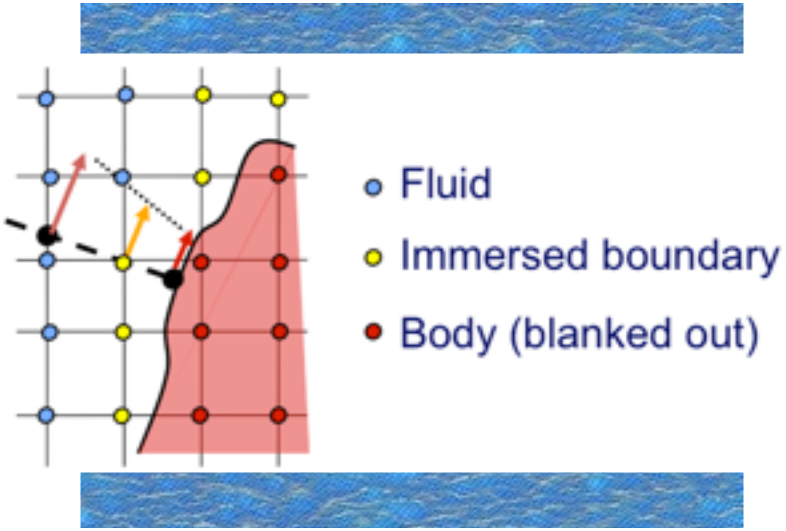
Advances in numerical algorithms

The **Virtual Flow Simulator** (VFS - Rivers®)

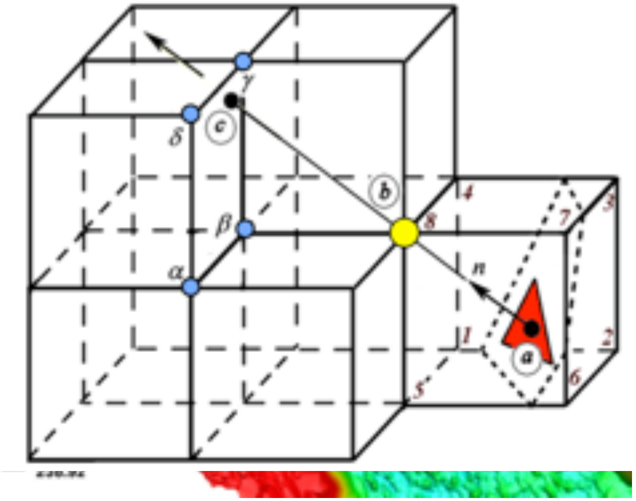
https://github.com/SAFL-CFD-Lab/VFS-Rivers

VFS-Rivers®: Large Eddy Simulation of turbulence in real-life waterways

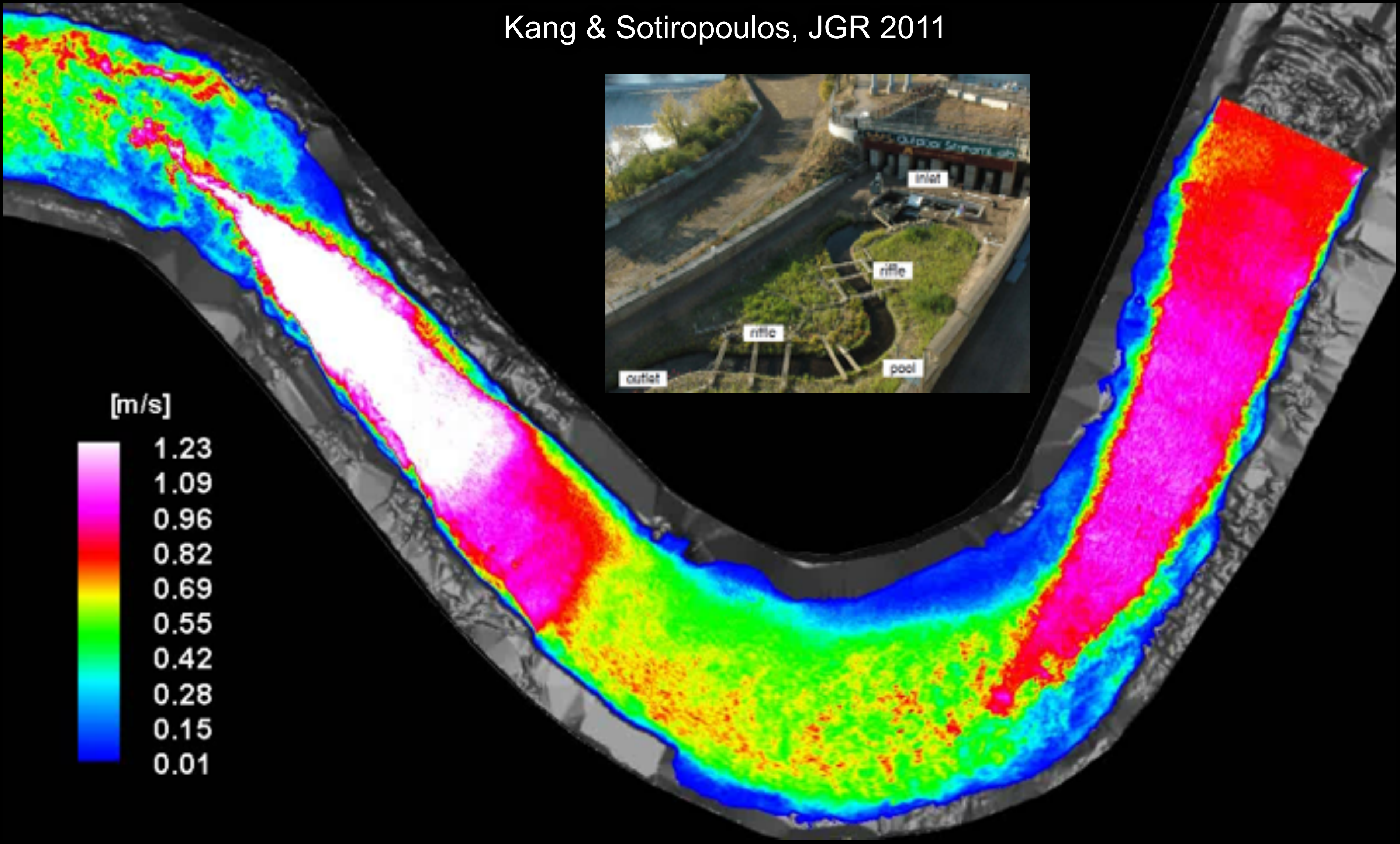
Kang et al, Adv. Water Res. 2010; Kang & Sotiropoulos JGR 2011, WRR 2012



- Curvilinear Immersed Boundary (CURVIB)
- Wall model to reconstruct velocity field at IB nodes
- 2nd order central differencing on a hybrid staggered/non-staggered grid
- Fractional-step algorithm: Jacobian-free Krylov solvers with Algebraic Multigrid
- Turbulence simulation and modeling:
    - ✓ DNS; LES; URANS
- Fluid-structure interaction (Borazjani et al., JCP, 2008)
- Fully parallelized with MPI



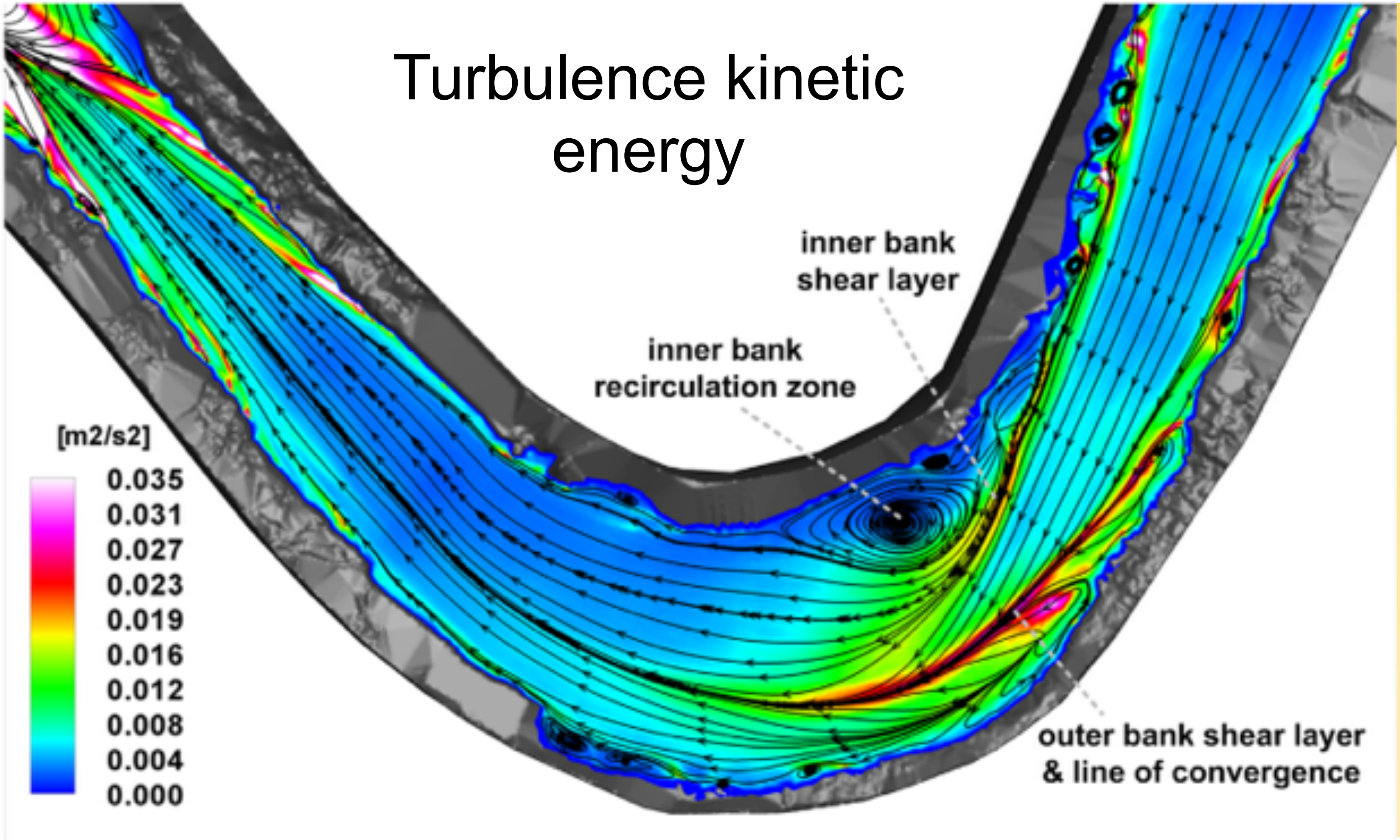
The SAFL Outdoor StreamLab: LES of bankfull flow



Kang & Sotiropoulos, JGR 2011

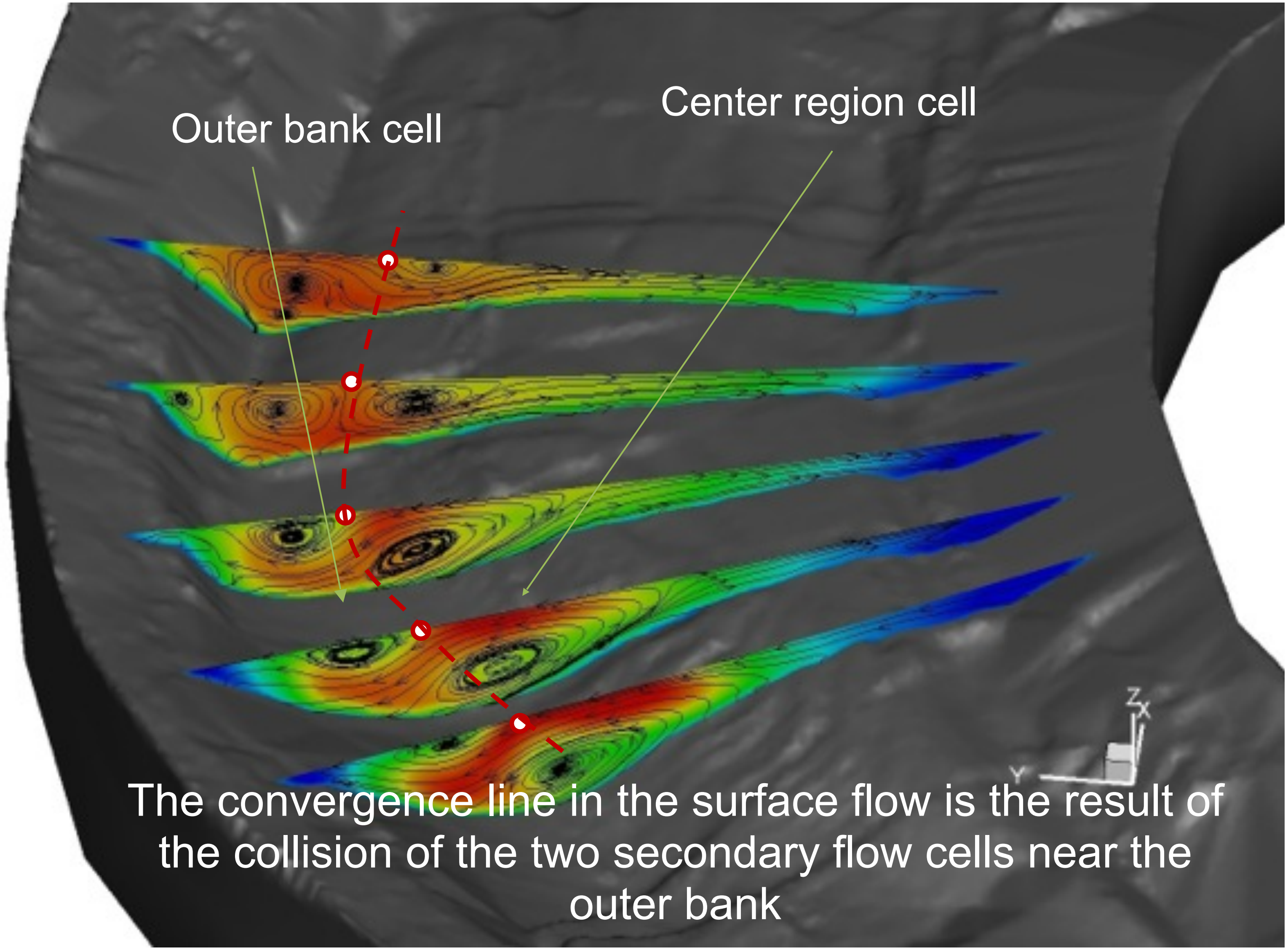
Flow physics in natural meander bends

Kang and Sotiropoulos, JGR – Earth Surface, 2011



Secondary flow in the pool

Kang and Sotiropoulos, JGR – Earth Surface, 2011

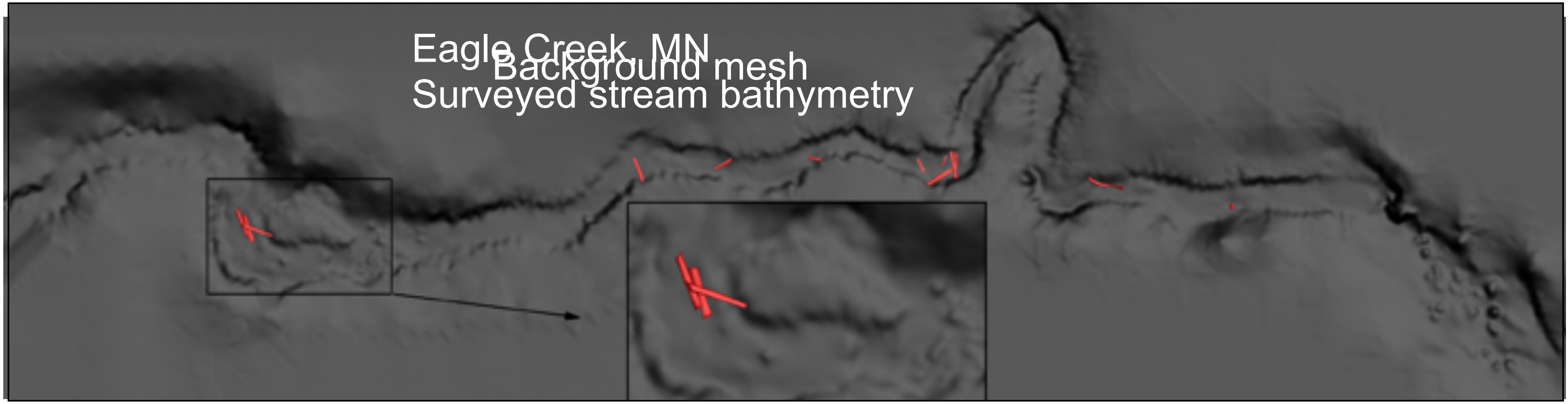


The convergence line in the surface flow is the result of the collision of the two secondary flow cells near the outer bank

Simulation-driven field experiments: Visualization of Surface Flow Convergence in the SAFL Outdoor StreamLab

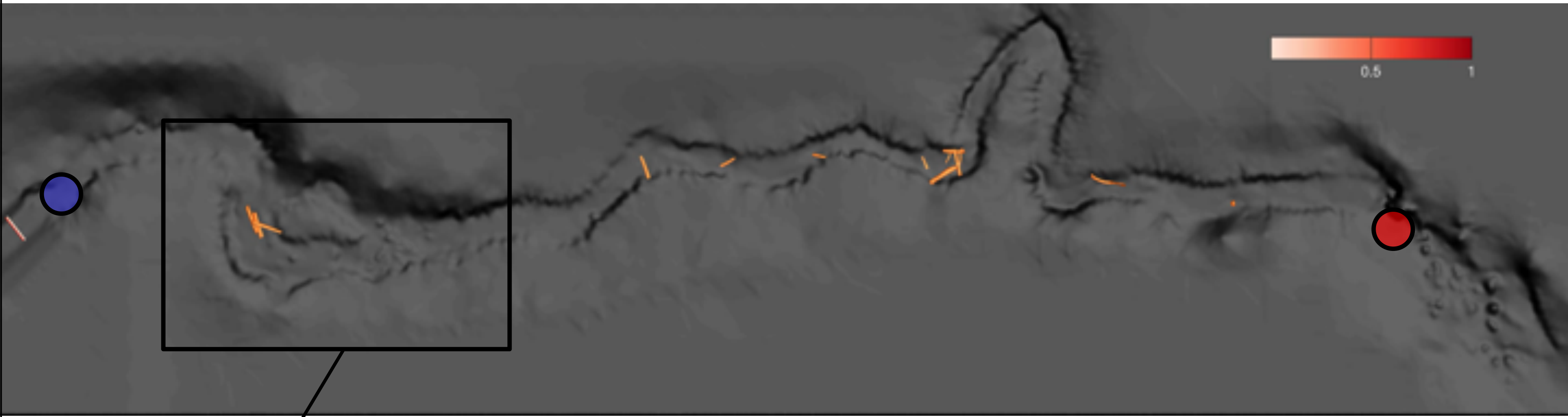
Data-driven simulations of turbulence in waterways

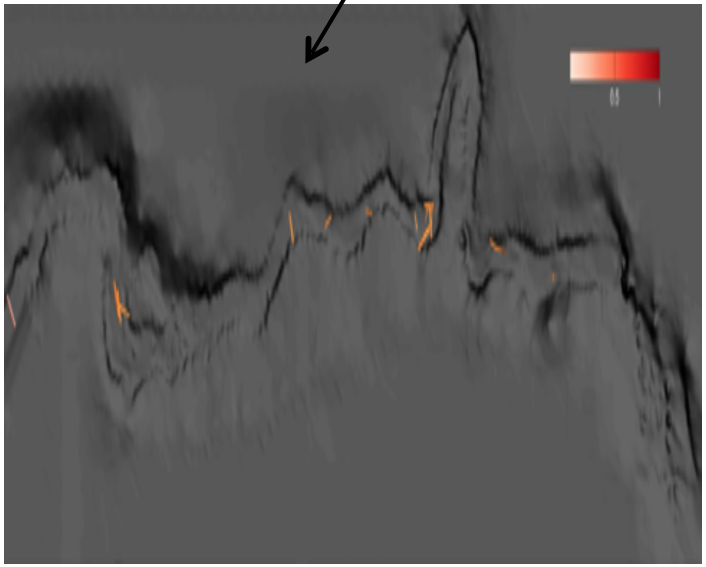
Khosronejad et al., JGR – Earth Surface 2016

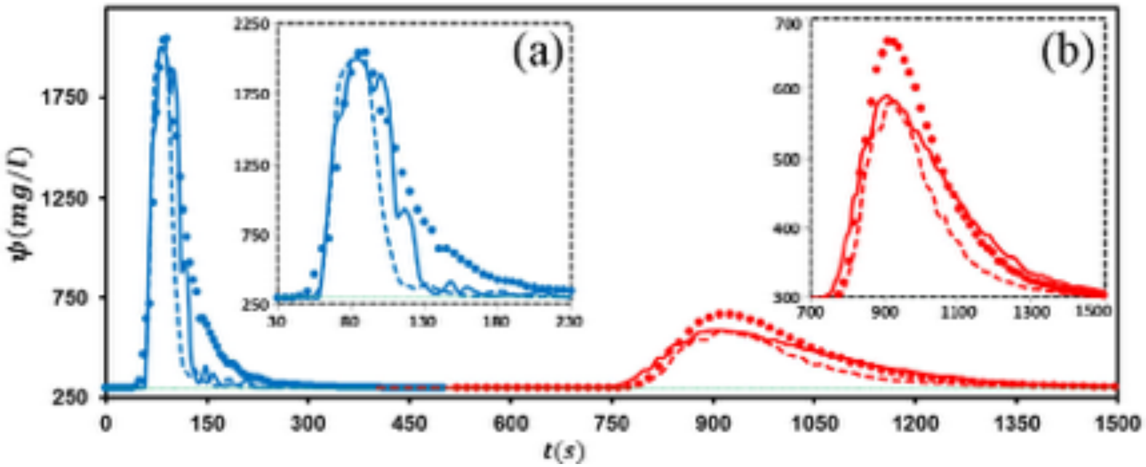


Data-driven simulations of turbulence and solute transport in waterways

Large-eddy simulation of solute transport in Eagle Creek, MN



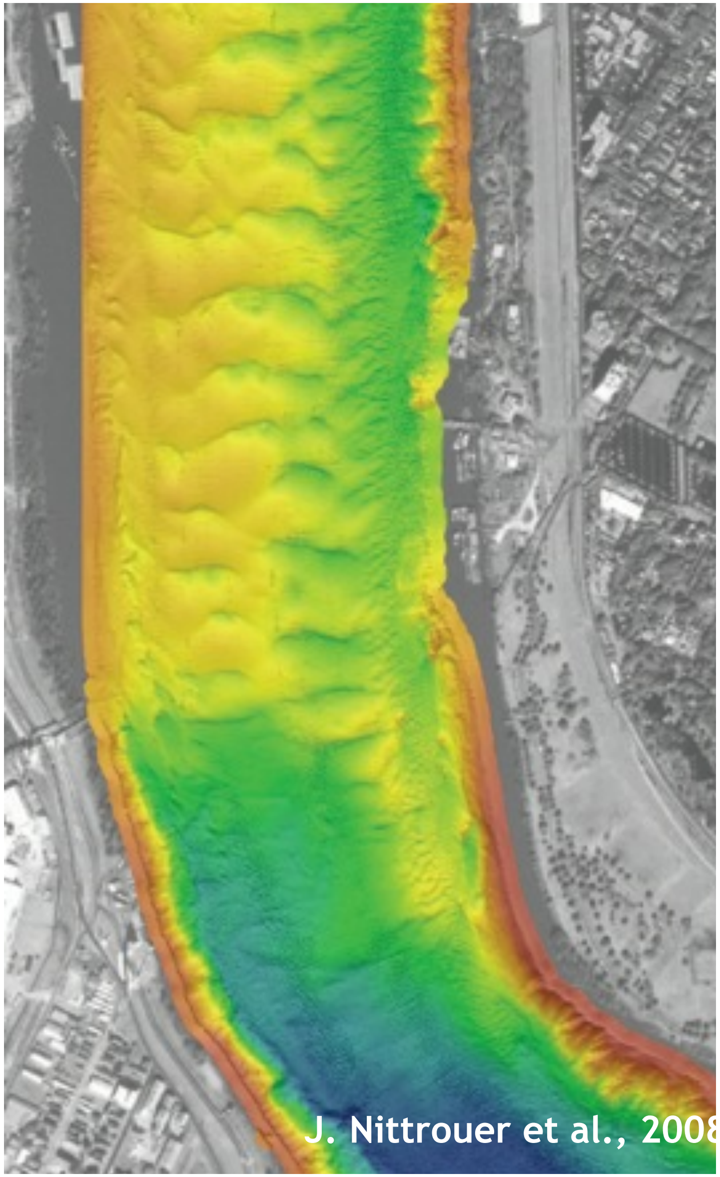




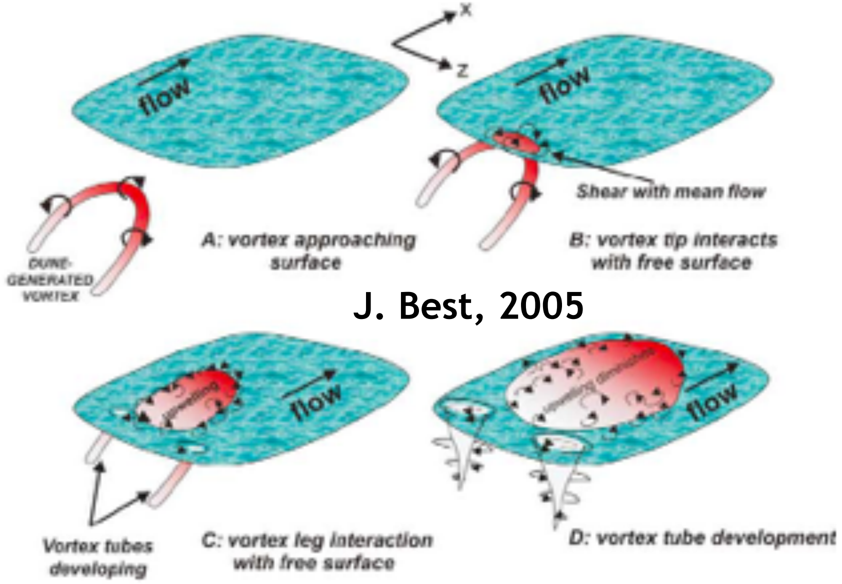
Sand waves in nature

Dunes after flooding in the Bonnet Carré Spillway in Louisiana
Image credit: Jeffrey Nittrouer

Dune-mitigated flow & transport phenomena



J. Nittrouer et al., 2008



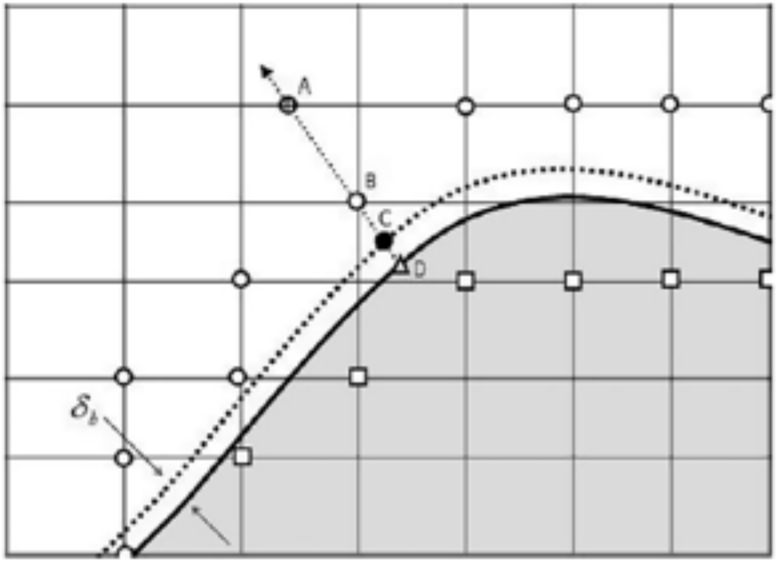
J. Best, 2005

- LES of turbulent flow over <u>frozen</u> dunes (e.g. Omidyeganeh and Piomelli, JFM 2013)
- Coupled models of small amplitude sand waves:
  Chu & Fringer, JGR 2010
  Escauriaza & Sotiropoulos, JGR 2011

Coupled models that can predict the onset & long-term evolution of <u>arbitrary amplitude</u> and <u>morphology</u> sand waves in <u>real-life</u> fluvial environments do not exist

Hydro-morphodynamic model

Khosronejad & Sotiropoulos, J. Fluid Mech., 2014

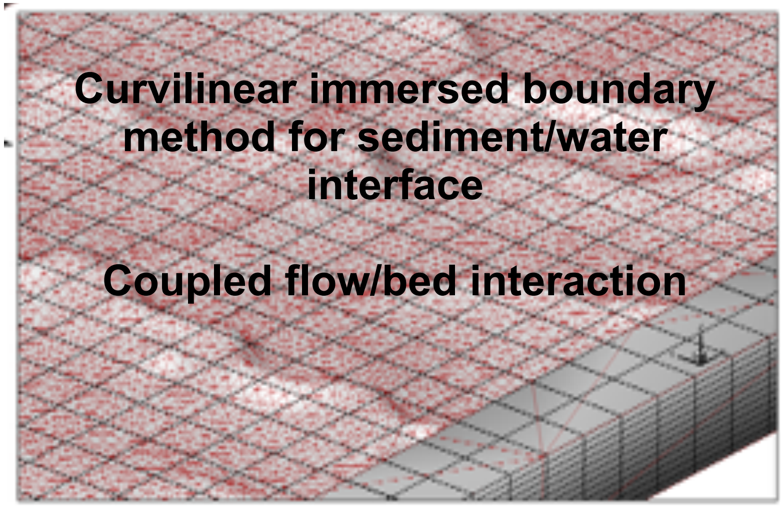


Hydrodynamic equations

Dilute mixture, Boussinesq assumption

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho_f}\nabla p + \frac{1}{\rho_f}\nabla\cdot\left(\tau_{visc} + \tau_{sgs}\right) + \frac{\varrho - \rho_f}{\rho_f}\boldsymbol{g}$$

$$\varrho = \rho_f(1-\psi) + \rho_s\psi$$



Curvilinear immersed boundary method for sediment/water interface

Coupled flow/bed interaction

Exner equation for bedload layer

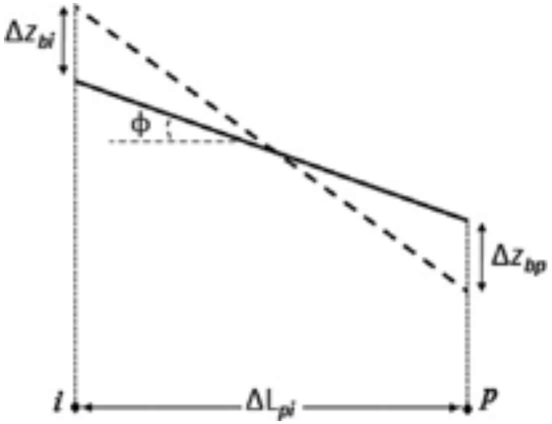
$$(1-\gamma)\frac{\partial z_b}{\partial t} = -\nabla\cdot\mathbf{q}_{BL} + D_b - E_b$$

Suspended load

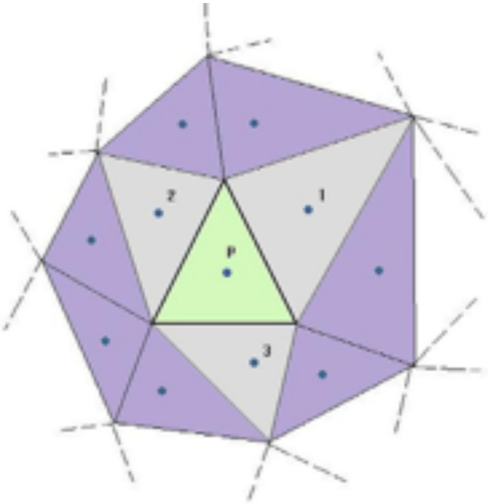
$$\frac{\partial\psi}{\partial t} + \nabla\cdot[(\boldsymbol{u}-\boldsymbol{w}_s)\psi] = \nabla\cdot[(\nu + \sigma^*\nu_{SGS})\nabla\psi]$$

Sand-slide model

- Solutions of the Exner equation could yield local bed slopes exceeding the material angle of repose
- In nature, local micro sand slides occur to prevent this from happening
- A numerical sand slide model: Mass-conservative correction of bed elevation calculated from the Exner equation



$$\frac{(z_{bp}+\Delta z_{bp})-(z_{bi}+\Delta z_{bi})}{\Delta l_{pi}} = \tan\phi$$



$$A_{hp}\cdot\Delta z_{bp} - \sum_{i=1,2,3} A_{hi}\cdot\Delta z_{bi} = 0$$

Sand waves in a laboratory flume

Venditti, Church & Bennett, J. of Geophysical Research, 2005

- Non-cohesive homogeneous particles - D_{50} = 0.5 *mm*
- U_{mean} = 0.5 m/s
- Flow depth: h = 0.115 m
- *Re* = 76,000
- Sand-wave characteristics:

Amplitude: Δ ~ 5cm
Wave length: λ ~ 10cm

Coupled hydro-morphodynamic LES of the Venditti et al. experiment

Khosronejad and Sotiropoulos, J. Fluid Mech., 2014

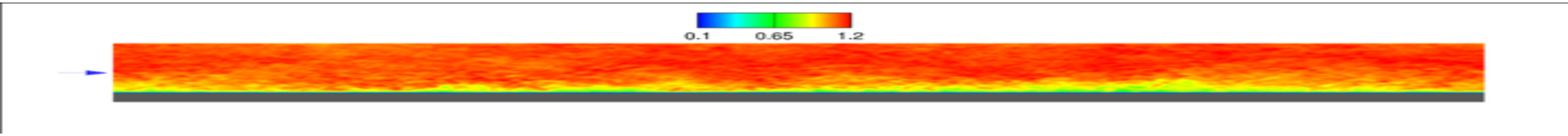
- Pre-computed (LES) fully developed channel flow fed at the inlet

- Sediment is re-circulated in the simulation as in the experiment

- Free surface is treated as a rigid lid

- Systematic grid refinement study: From 2×10^7 to 8×10^7 grid nodes

Flow/sand-wave dynamics



Instantaneous velocity magnitude

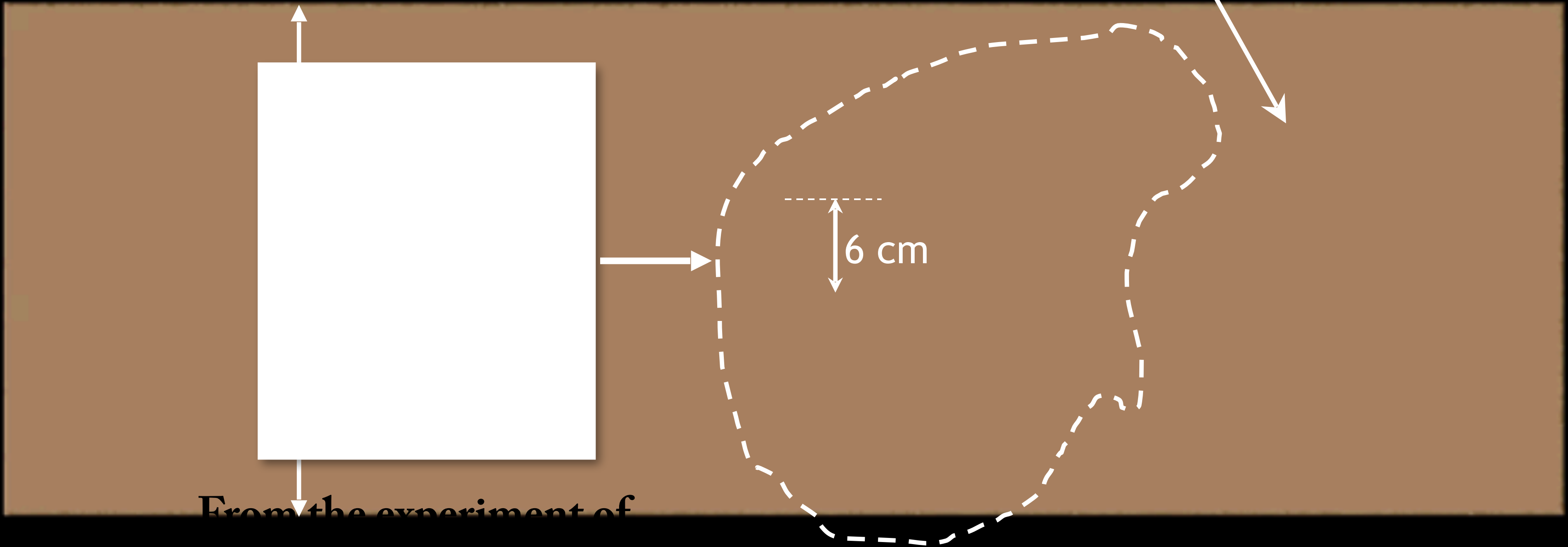
Suspended sediment concentration

Simulated temporal evolution of the mobile-bed

Transition to 3D pattern

Sand wave initiation

Merging process

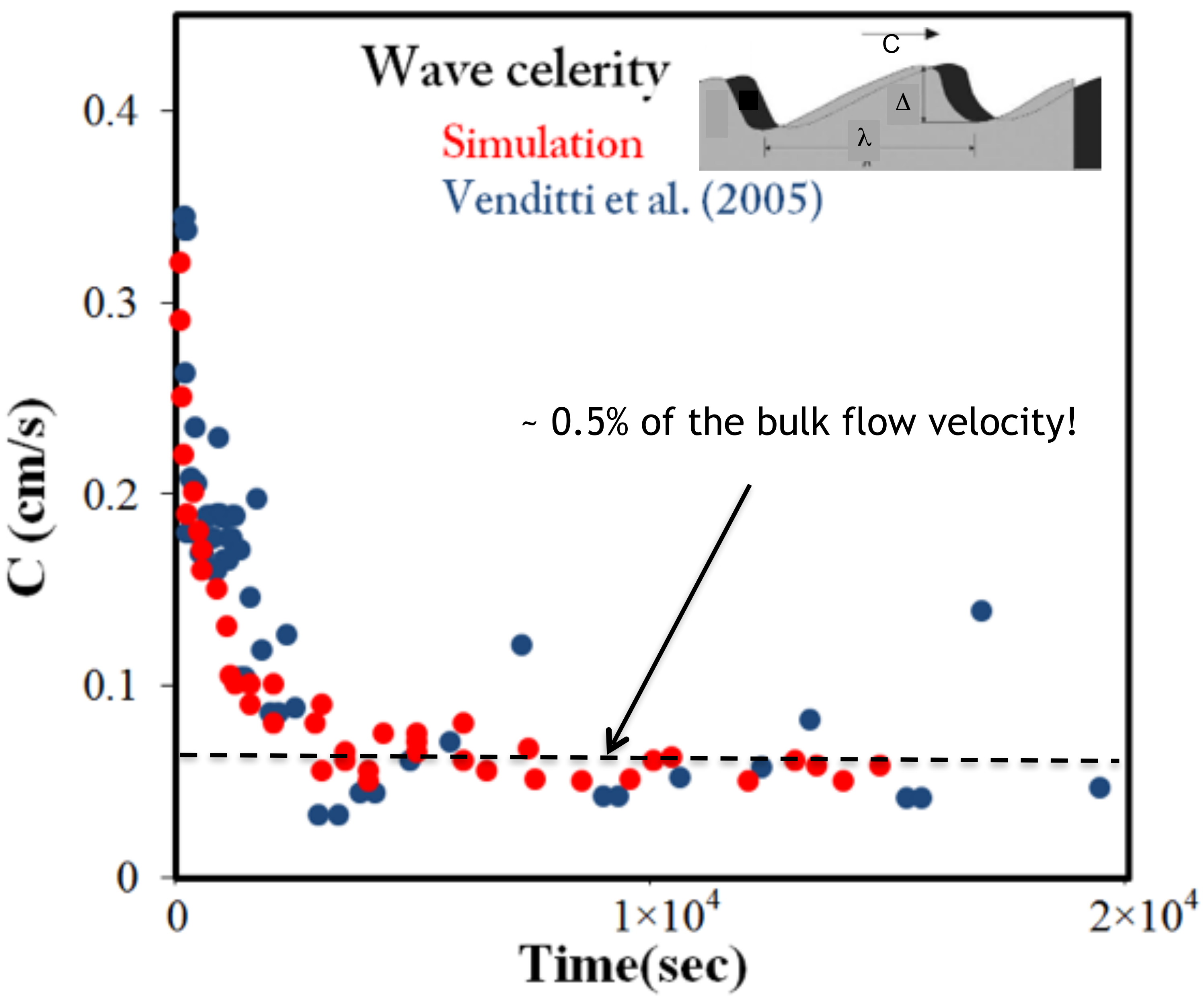


From the experiment of

0 < t < 3600 sec

t = 3600 sec

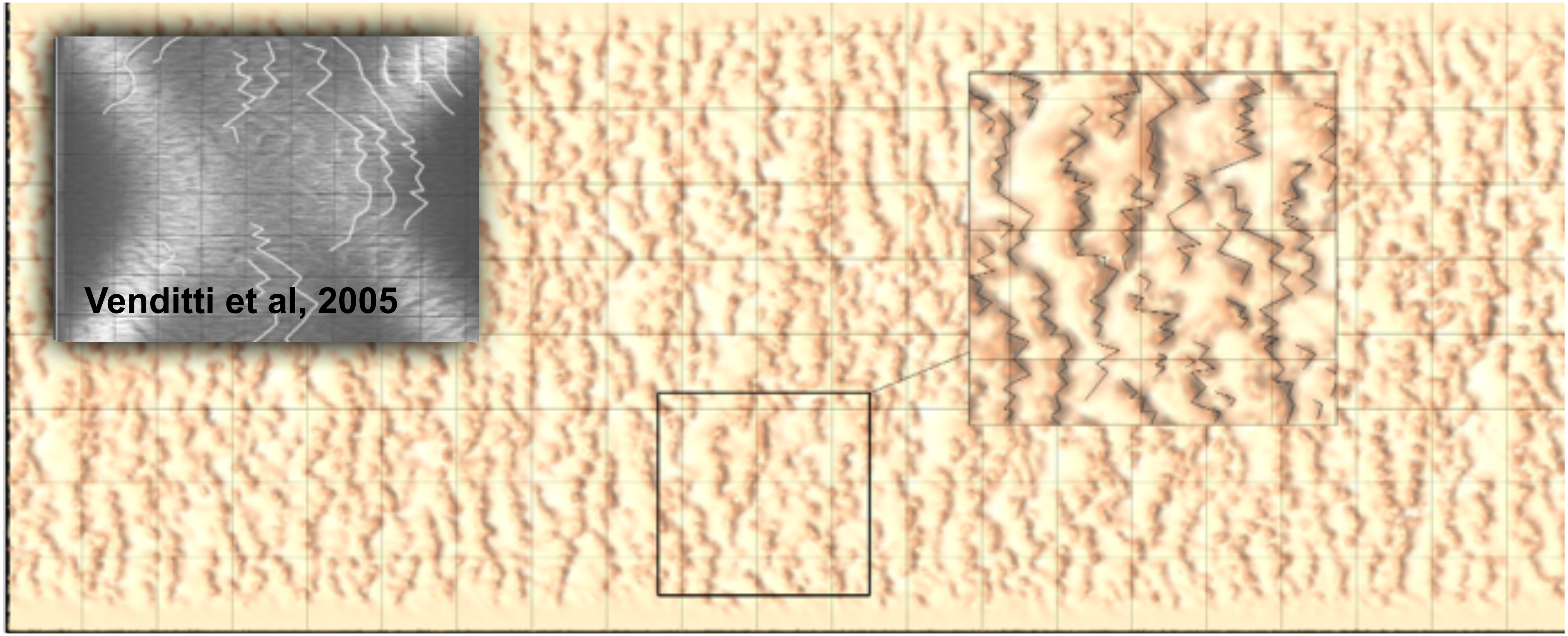
Comparisons with experiments



~ 0.5% of the bulk flow velocity!

Simulated sand waves

Initial stages of bed instability



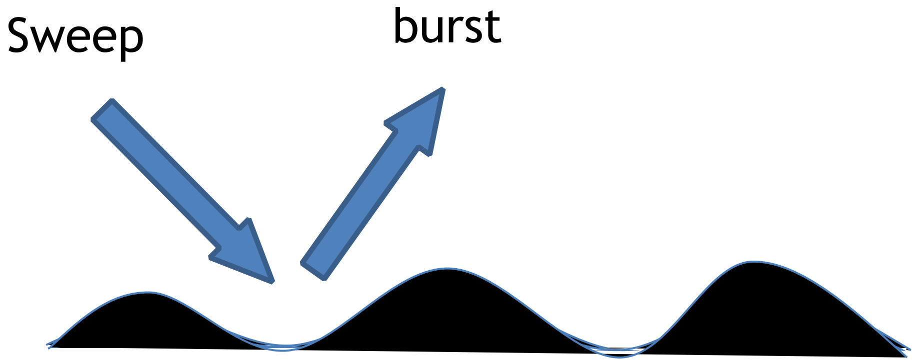
Venditti et al, 2005

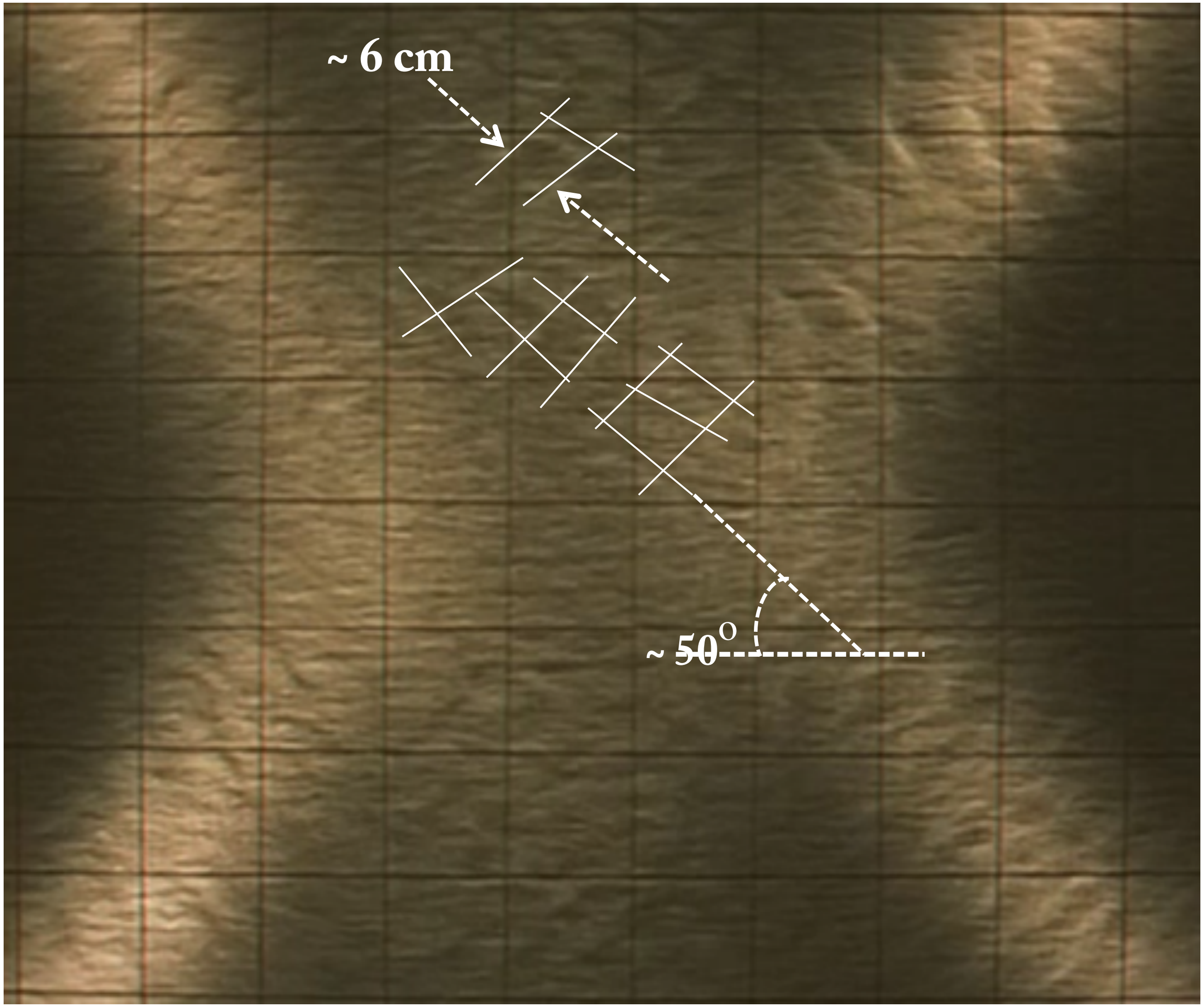
[illegible]

How do sand waves originate?

It has long been hypothesized that sand waves initiate by the action of turbulent sweeps over mobile-bed

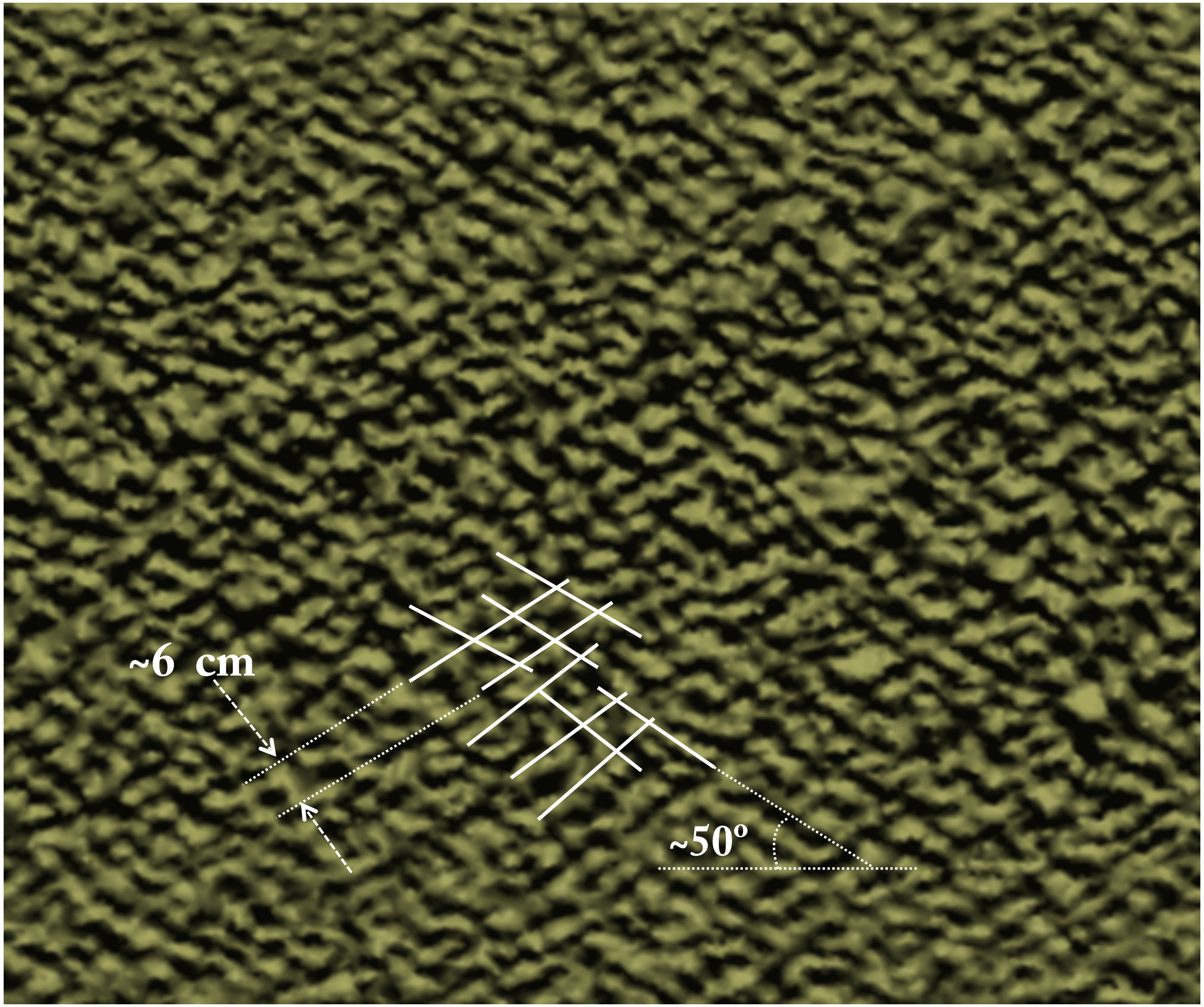
Grass 1970,1971; Coleman & Melville 1994; Best & Kostaschuk 2002; Venditti et al, 2005





They take the form of oblique linear striations with an amplitude of ~0.1 cm ($2d_{50}$), wavelength of 4-7 cm, forming angles with the centerline in the range of 40º and 60º

In the experiment of Venditti & Church (2005) distinct *cross-hatch patterns appear spontaneously on the initially flat sand bed* shortly after the start of the flow



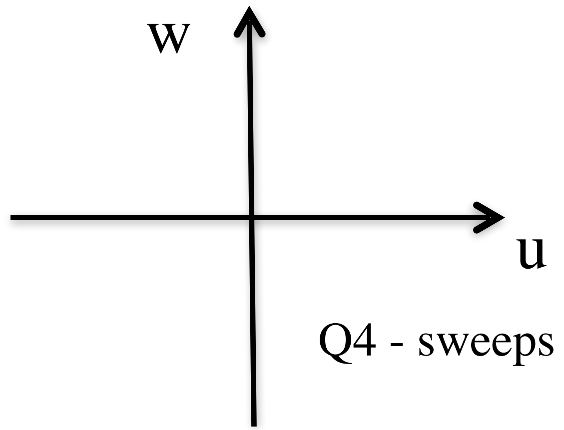
The simulated sand-waves at t=2 sec also take the form of oblique linear striations with an amplitude of ~0.1 cm (2d_{50}), wavelength of 4-7 cm; forming angles with the centerline in the range of 45º and 55º

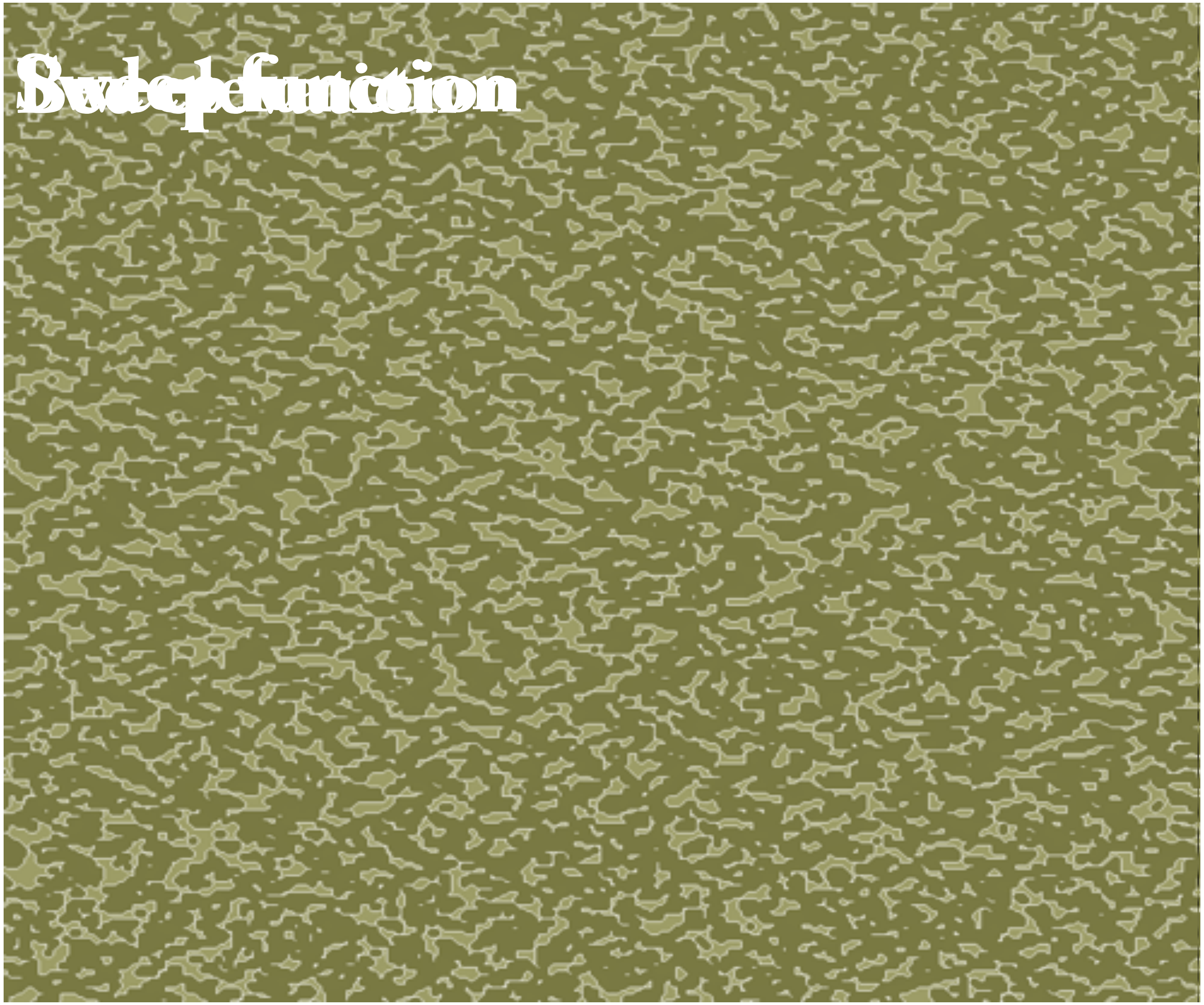
Identical cross-hatch patterns also appear in the simulated bed shortly after the start of the coupled hydro-morphodynamic simulation

The sweep detection function

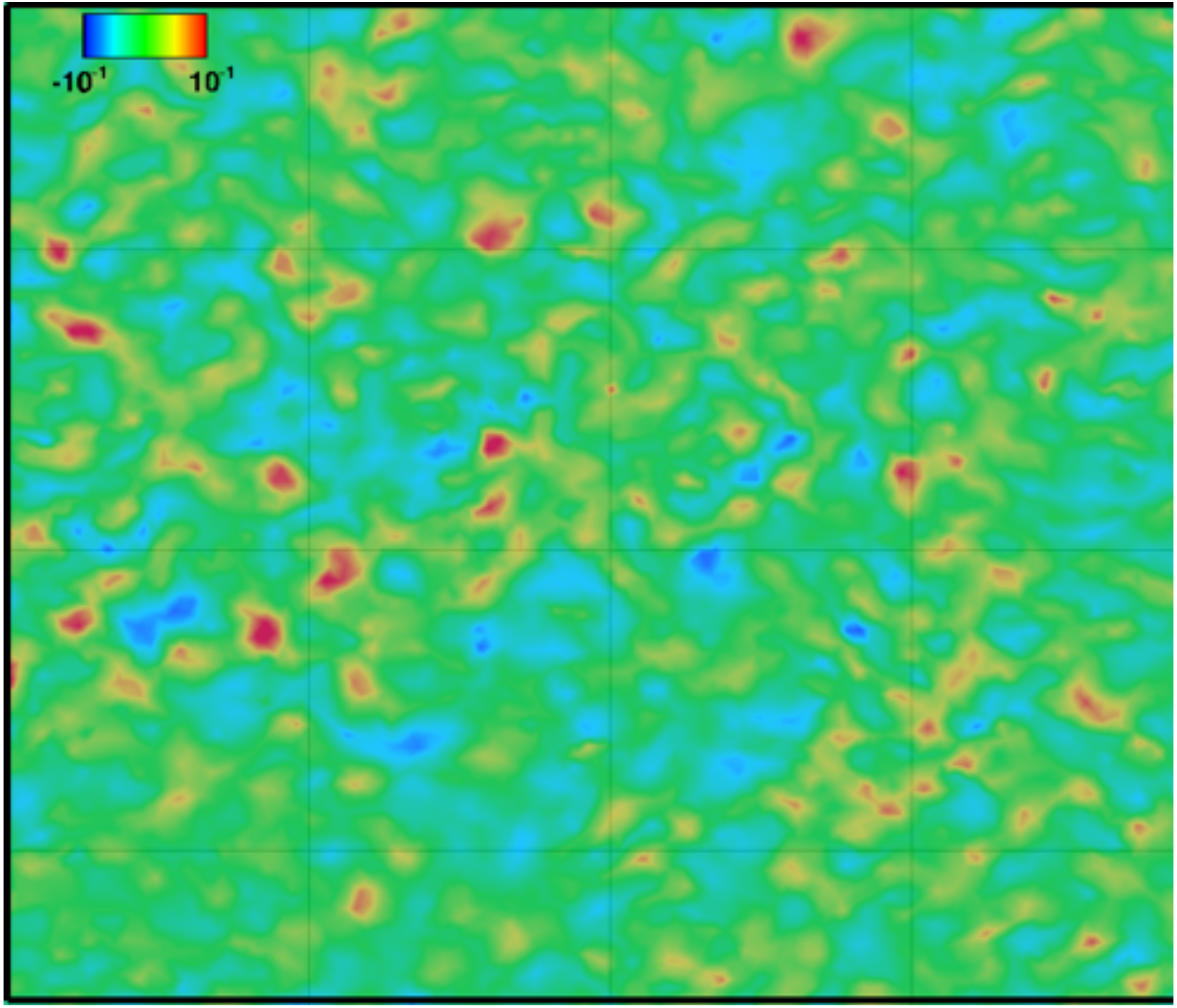
Identify instantaneous Q4 events:

$$F_s = \begin{cases} 1 & \text{if } u' > 0 \text{ and } w' < 0, \\ 0 & \text{elsewhere.} \end{cases}$$



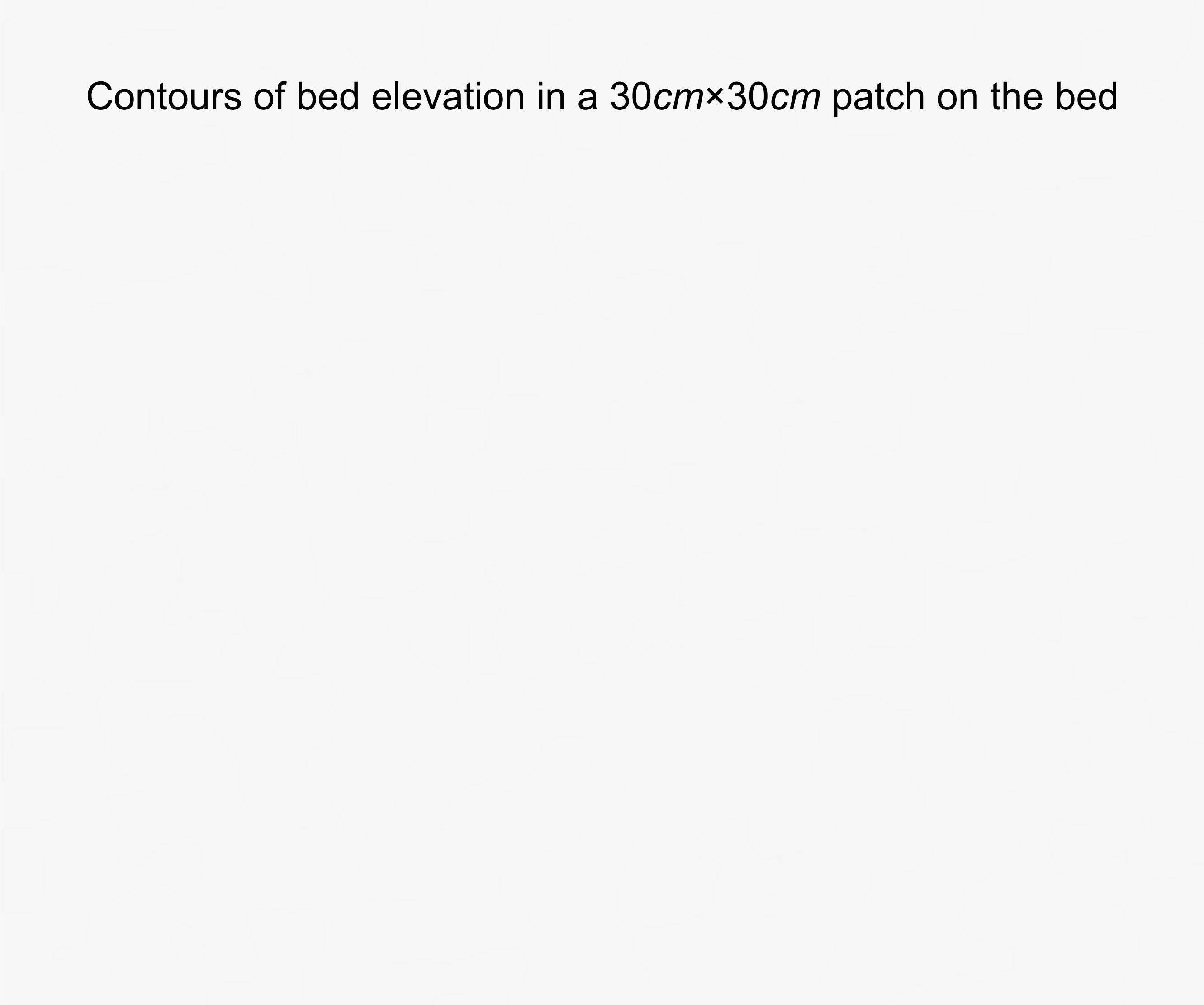


The spatial structure of Q4 events at the start of bed instability exhibits cross-hatch patterns correlating in length, shape and orientation with marks on the bed



Wall shear stress fluctuations exhibit similar cross-hatch patterns

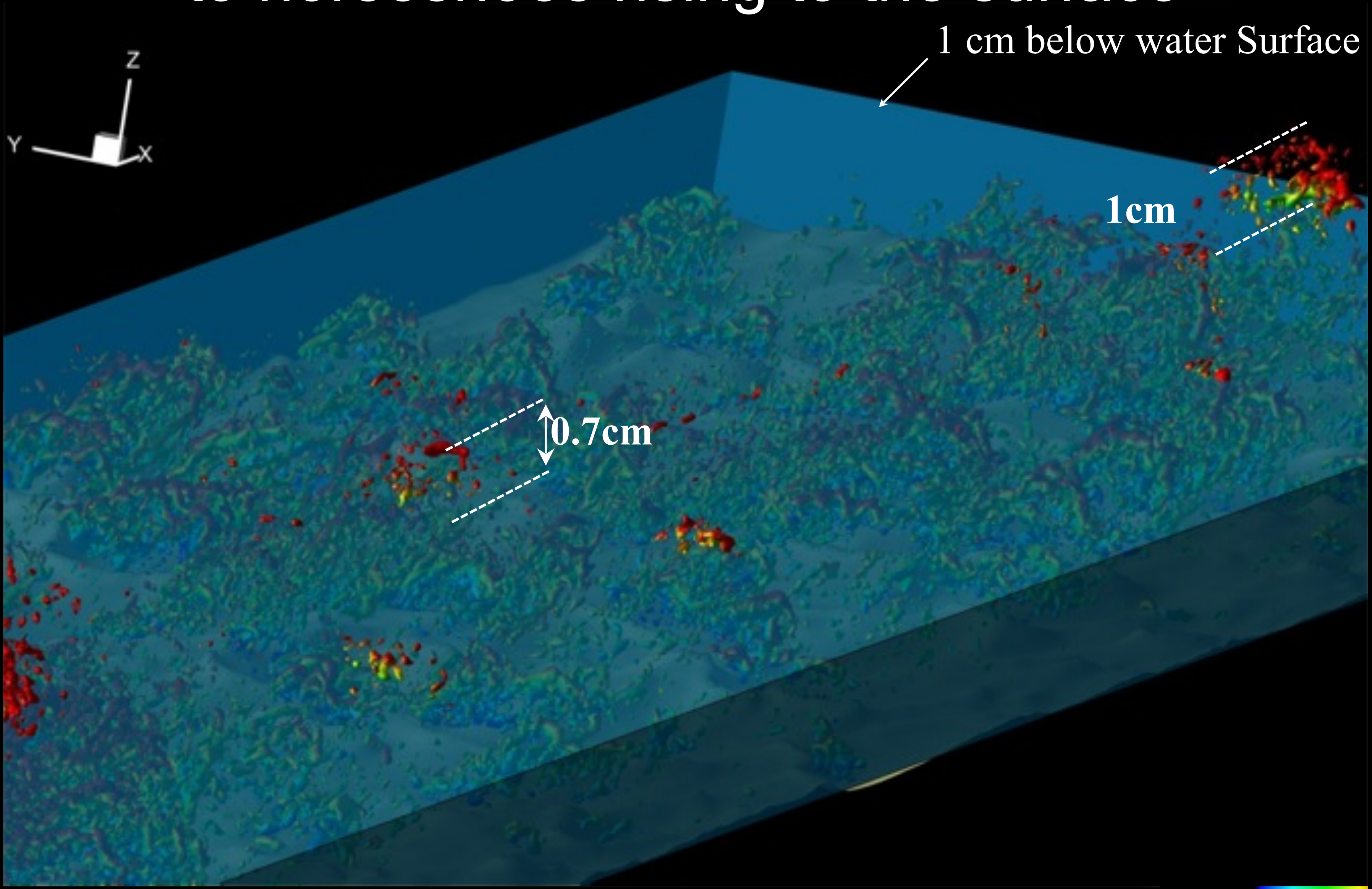
Micro-scour events originate within sweeps where the local shear stress increases as the results of momentum transfer by sweeping motions



Contours of bed elevation in a 30*cm*×30*cm* patch on the bed

Self-organize by catching up with bigger & slower neighbors

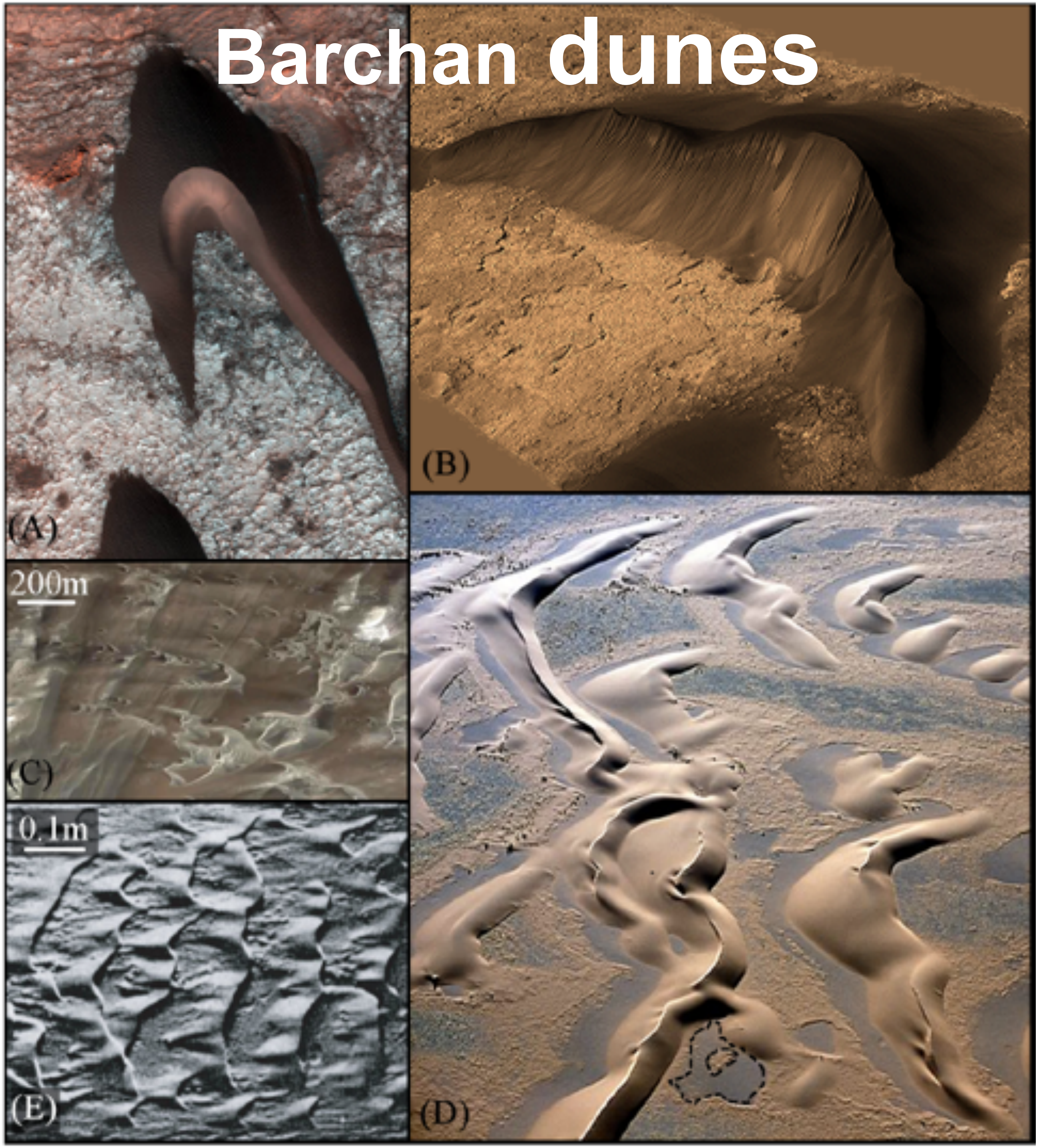
From cross-hatch marks to 3D dunes giving rise to horseshoes rising to the surface



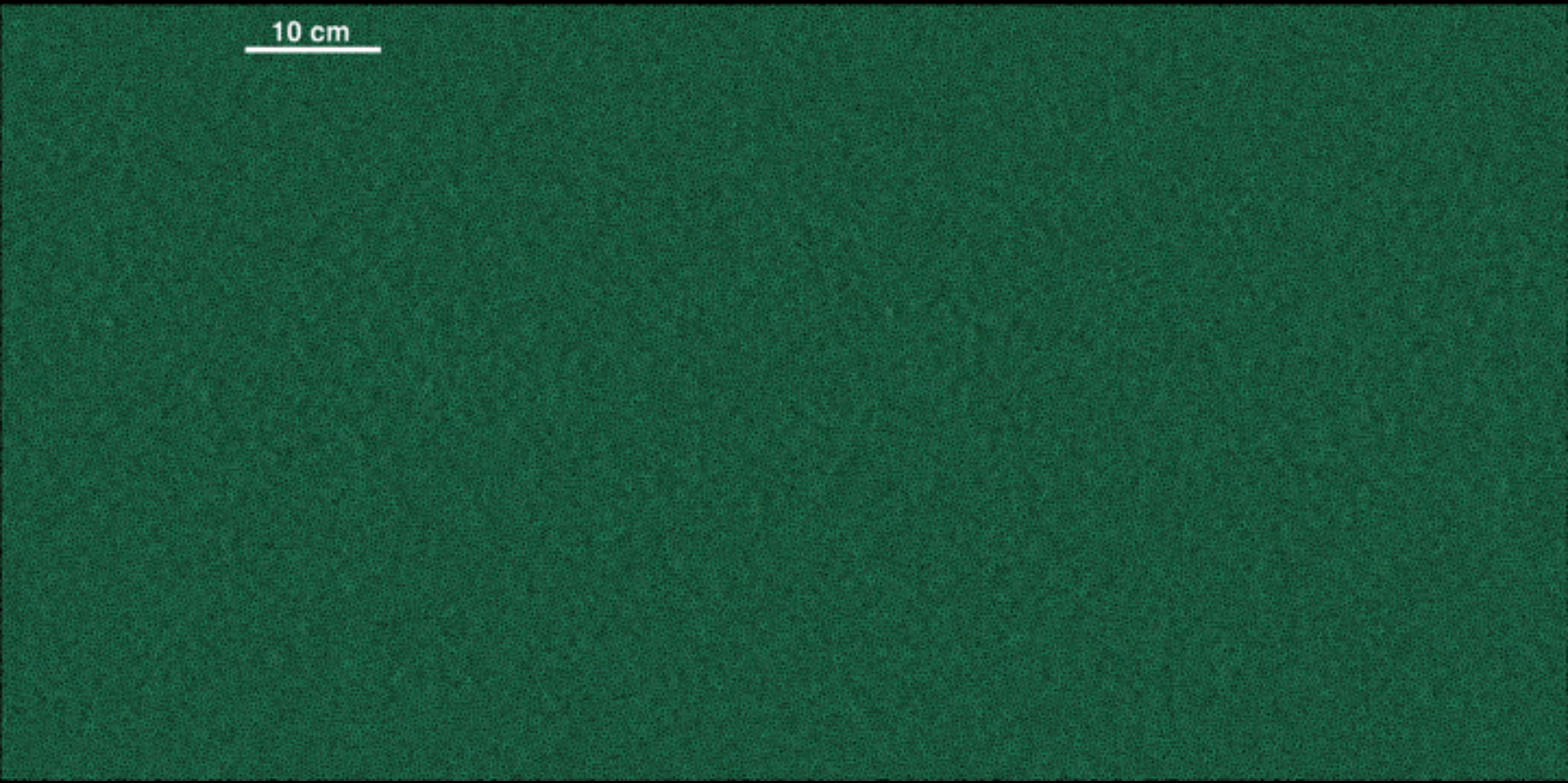
Sand wave to 3D pattern

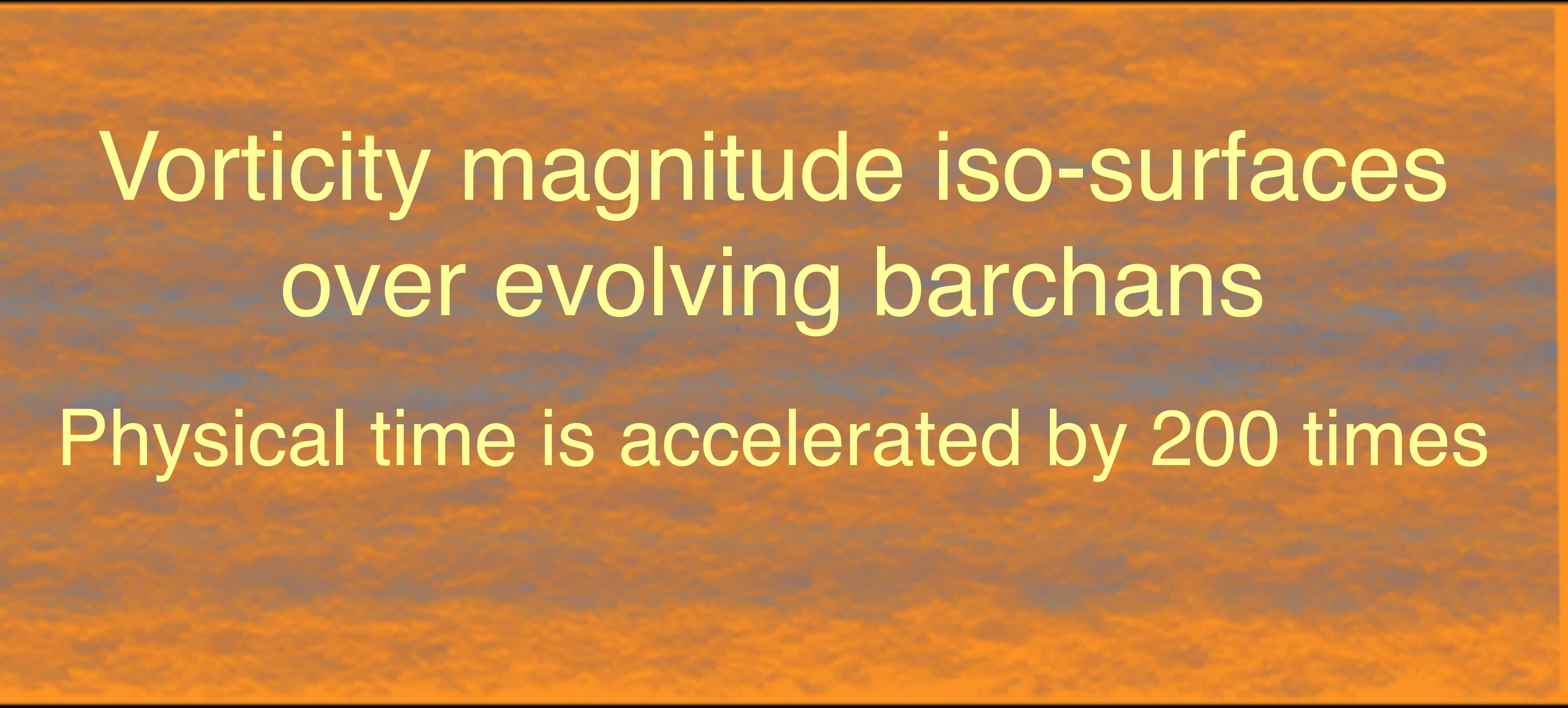
300 < t < 400 sec

Barchan dunes



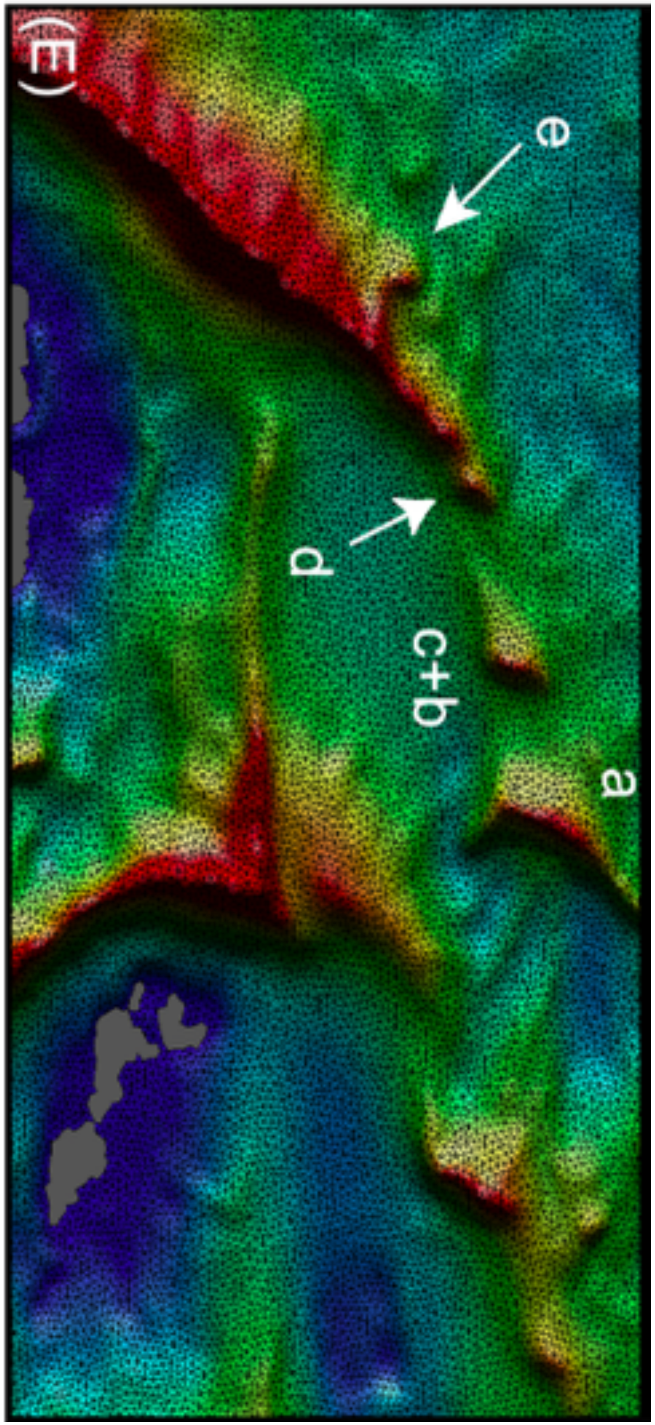
Coupled hydro-morphodynamic LES of barchan dunes in a turbulent open channel flow

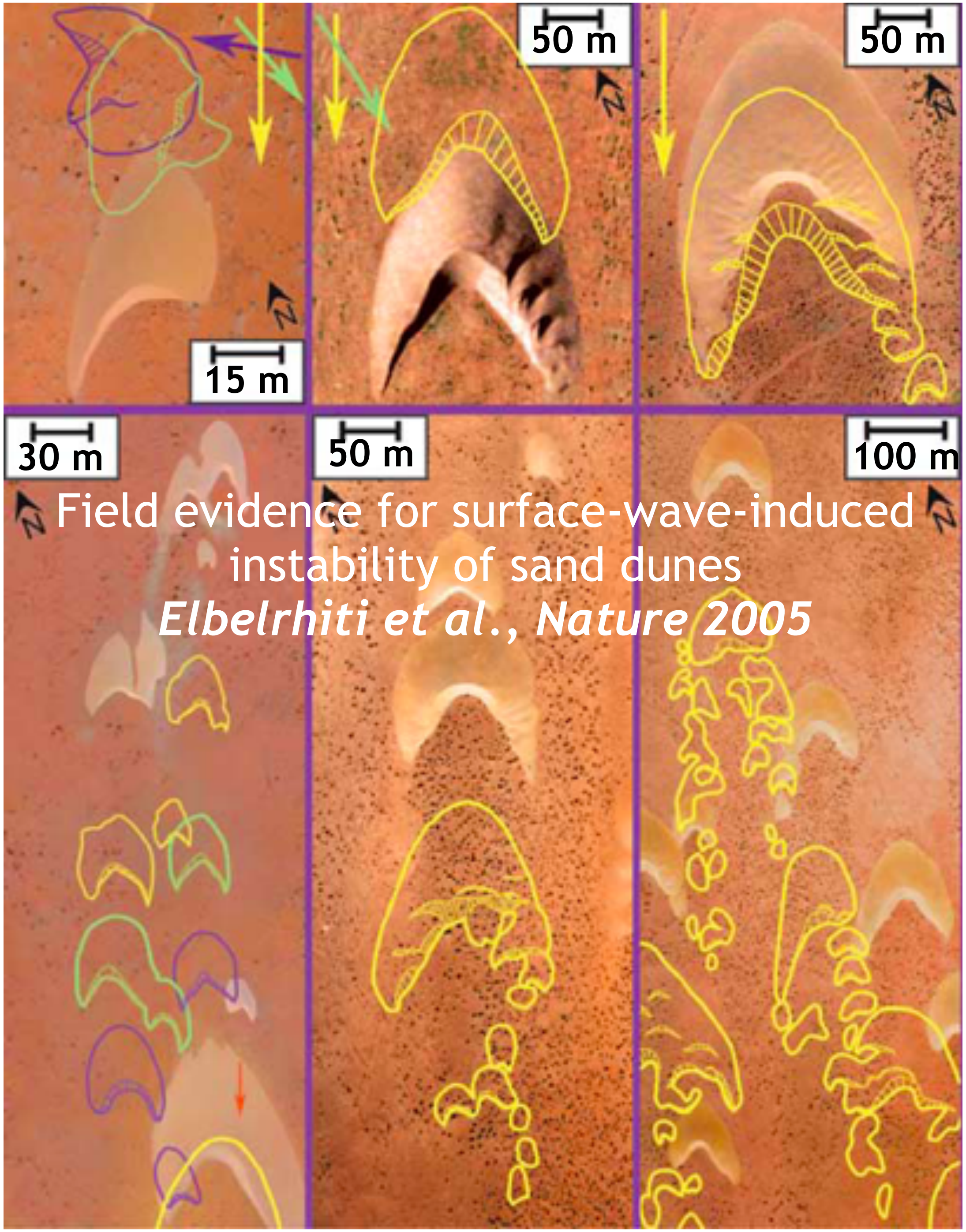




Vorticity magnitude iso-surfaces over evolving barchans

Physical time is accelerated by 200 times

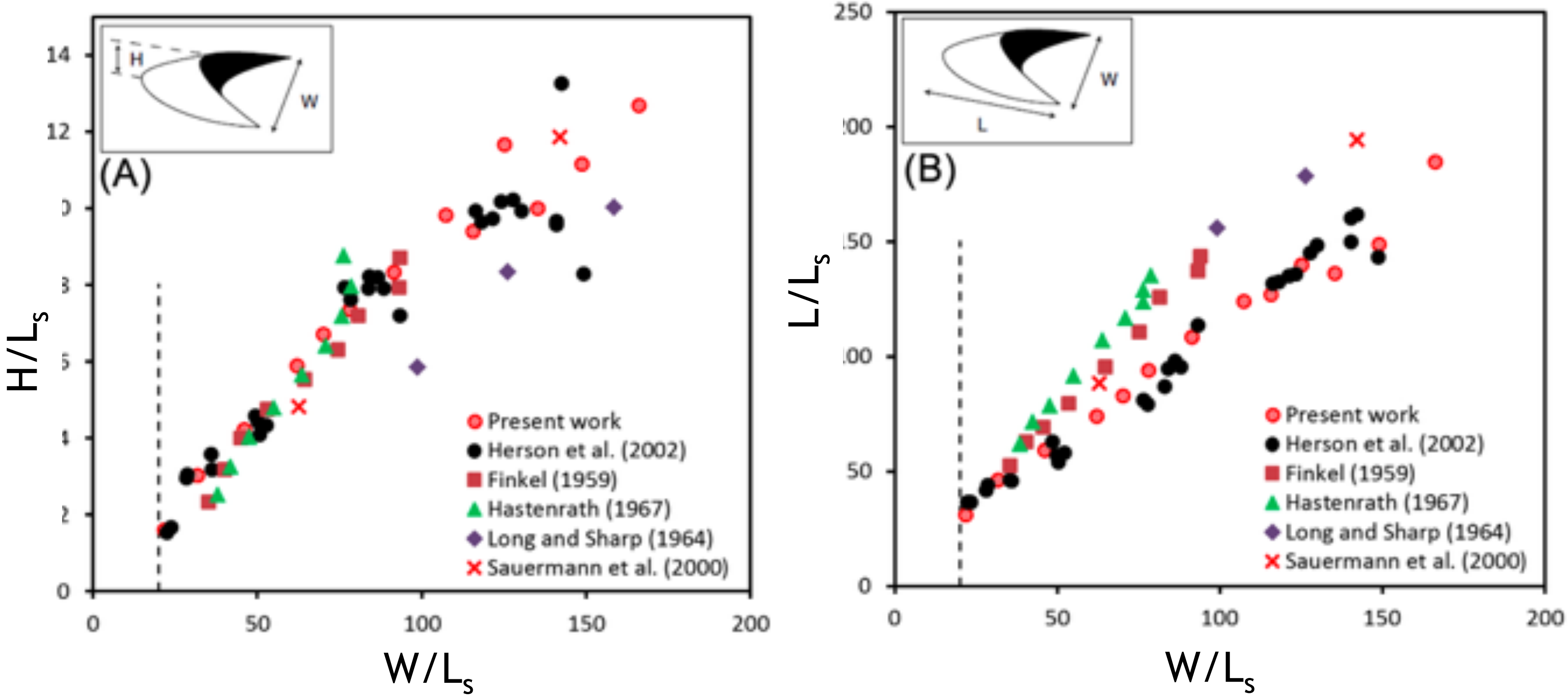




Field evidence for surface-wave-induced instability of sand dunes

Elbelrhiti et al., Nature 2005

Simulated dunes are similar to those observed in nature



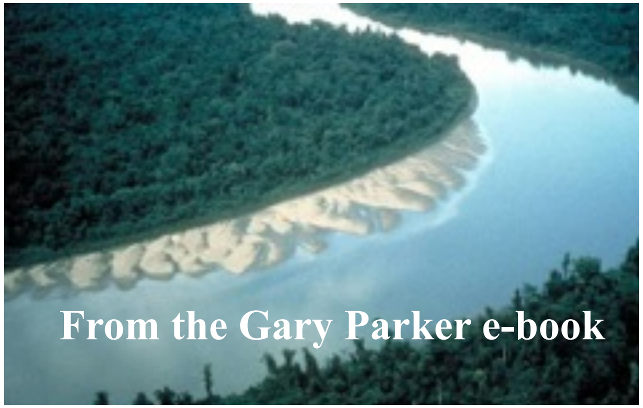
$$L_s = \frac{\rho_s}{\rho_f} d_{50}$$

P. Hersen et al., "Relevant length scale of barchan dunes," Phys. Rev. Letters, 2002.

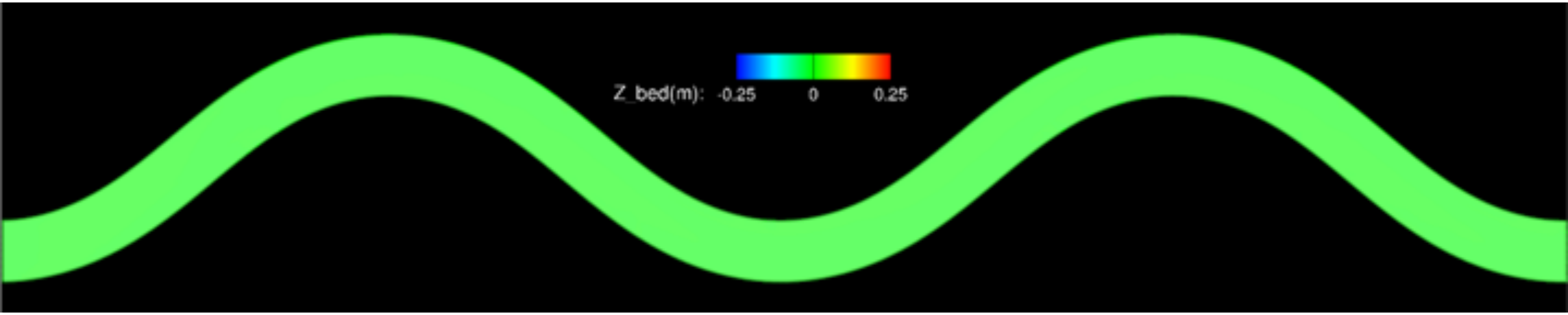
Dune migration in large rivers

Khosronejad et al., Adv. Water Res. Res., 2014

Computed dunes:
Δ ~ 0.5 – 1.5m
λ ~ 10 – 30m


From the Gary Parker e-book

Unsteady RANS simulation of dune migration in a large meandering river



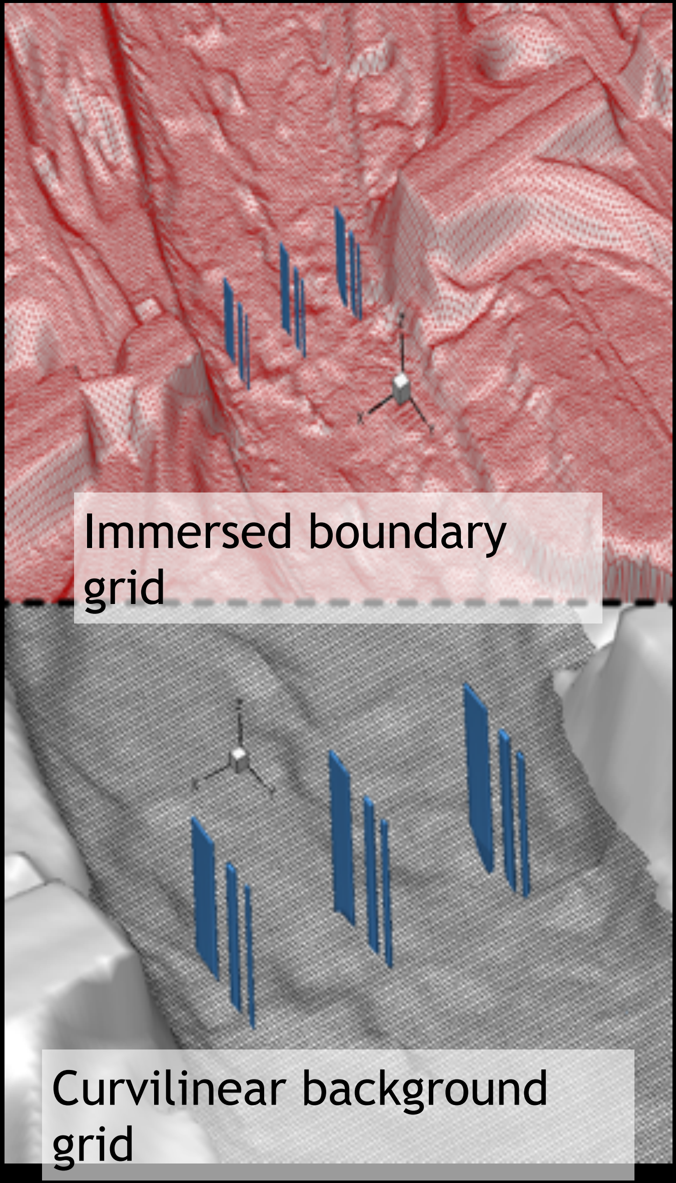

The SAFL Outdoor StreamLab

Data-driven simulations of extreme flooding in the Upper Mississippi River

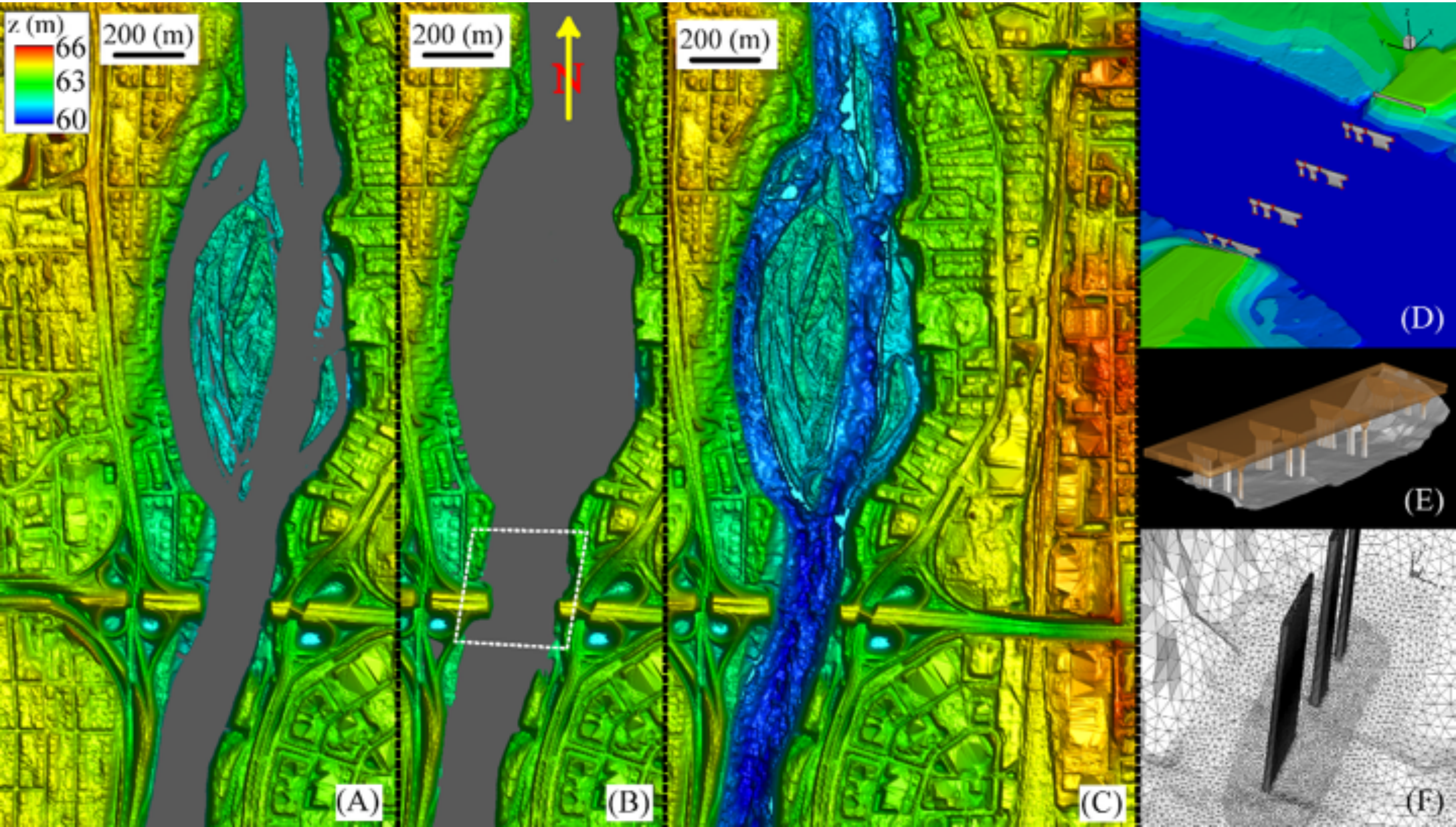
- **Objective:** Finding maximum scour depth under extreme flood conditions of **100 and 500 year-floods**
- **Source of geometrical data:** LiDAR; Sonar onboard a boat; Laser scanner
- **Sources of flow field data for model validations**: Acoustic Doppler Current Profile (ADCP) onboard a boat

Construction of the Digital Terrain Model

- Floodplain terrain elevation
- River bathymetry **below** water surface
- Water depth for flood conditions
- Bridge piers geometrical data
- Combine all to obtain the digital terrain map & computational grid

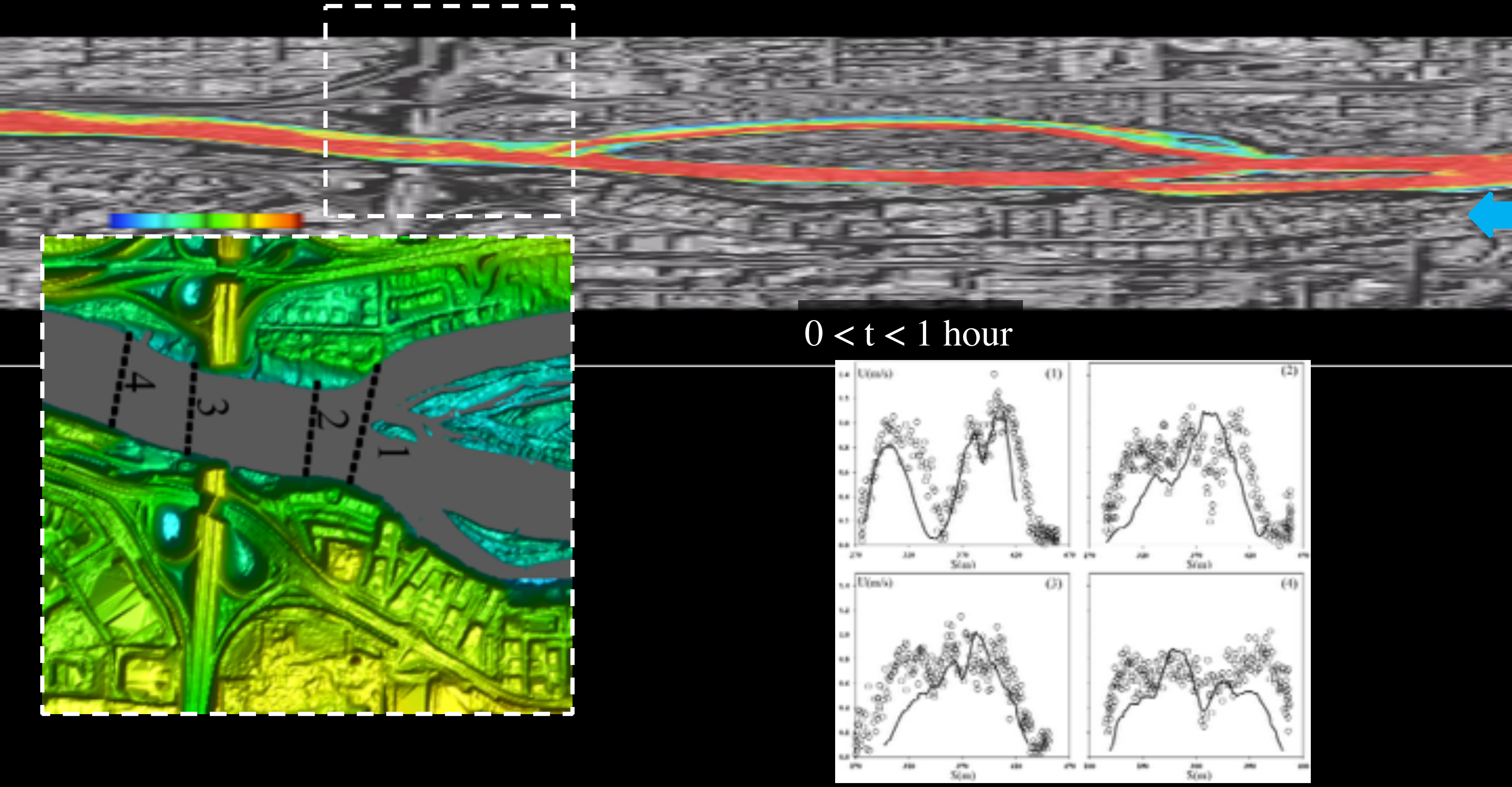


High-resolution DTM by fusing a variety of data sets



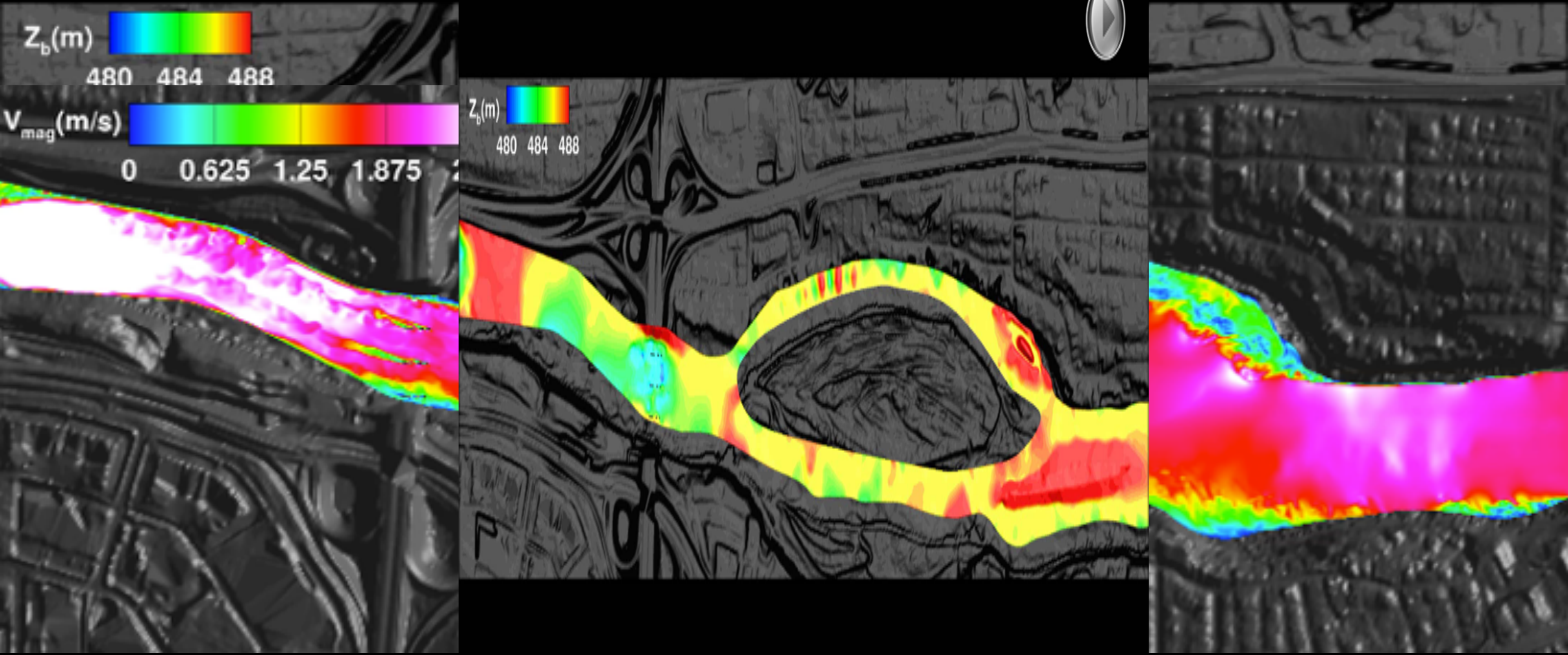
Validating the flow solver: base-flow condition

T. Le, A. Khosronejad, & F. Sotiropulos, *Adv. Water Res.*, In Review, 2016



0 < t < 1 hour

Hydrodynamics & morphodynamics of a 100-year flood event

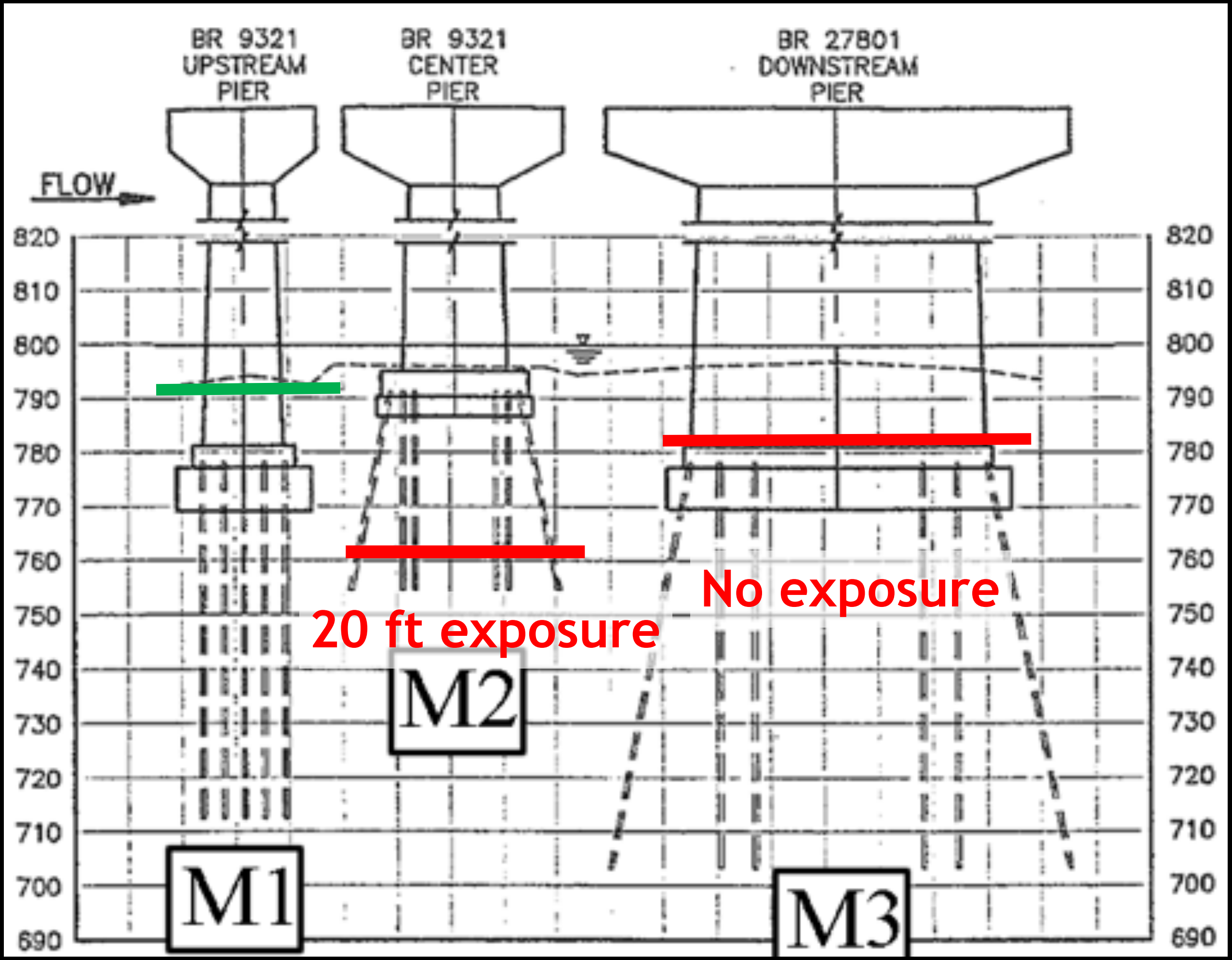


Simulating bridge foundation scour at field scale

Translating the simulation results for practitioners & engineers

Pier 2

500-year flood

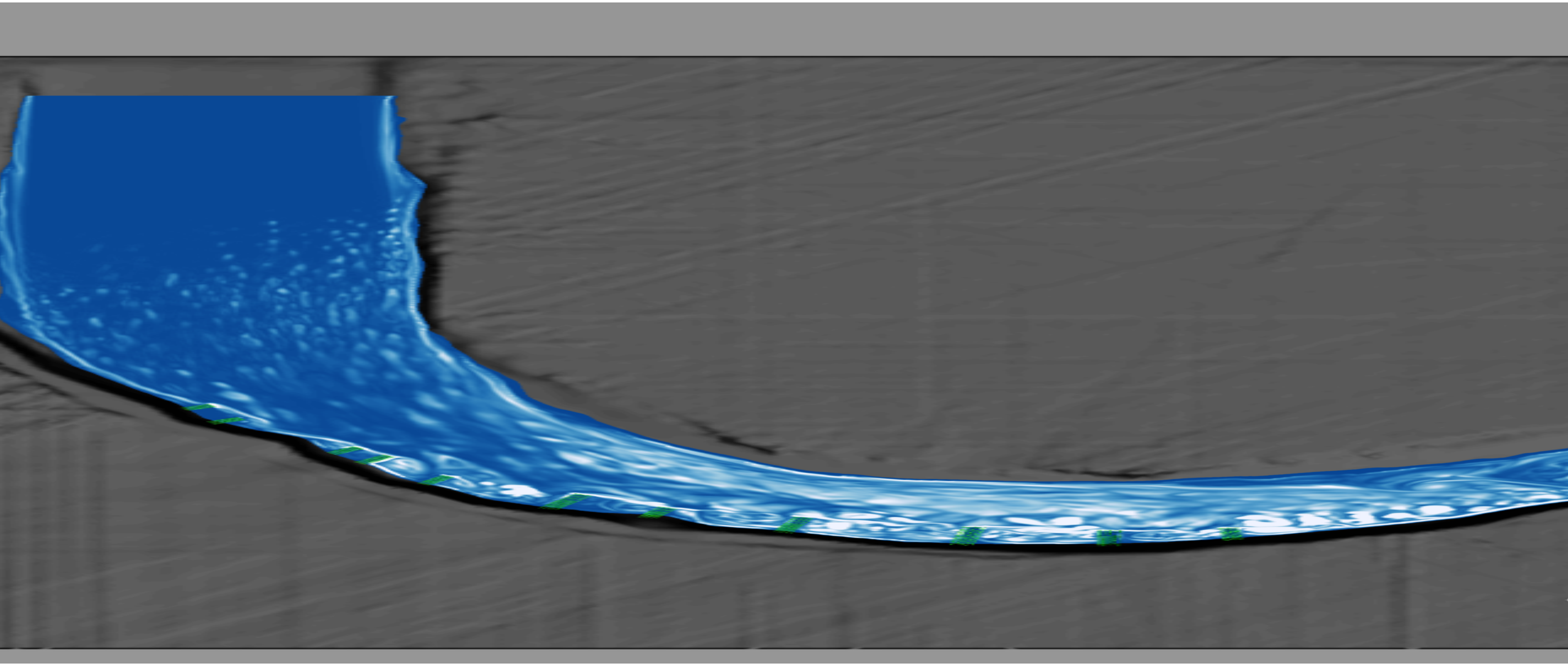


Rio de madre de Dios, Puerto Maldonado, Medre de Dios, Peru

Courtesy: J. Kuroiwa, Luis F. Castro, UNI de Peru

Approaching by ~12 m/year

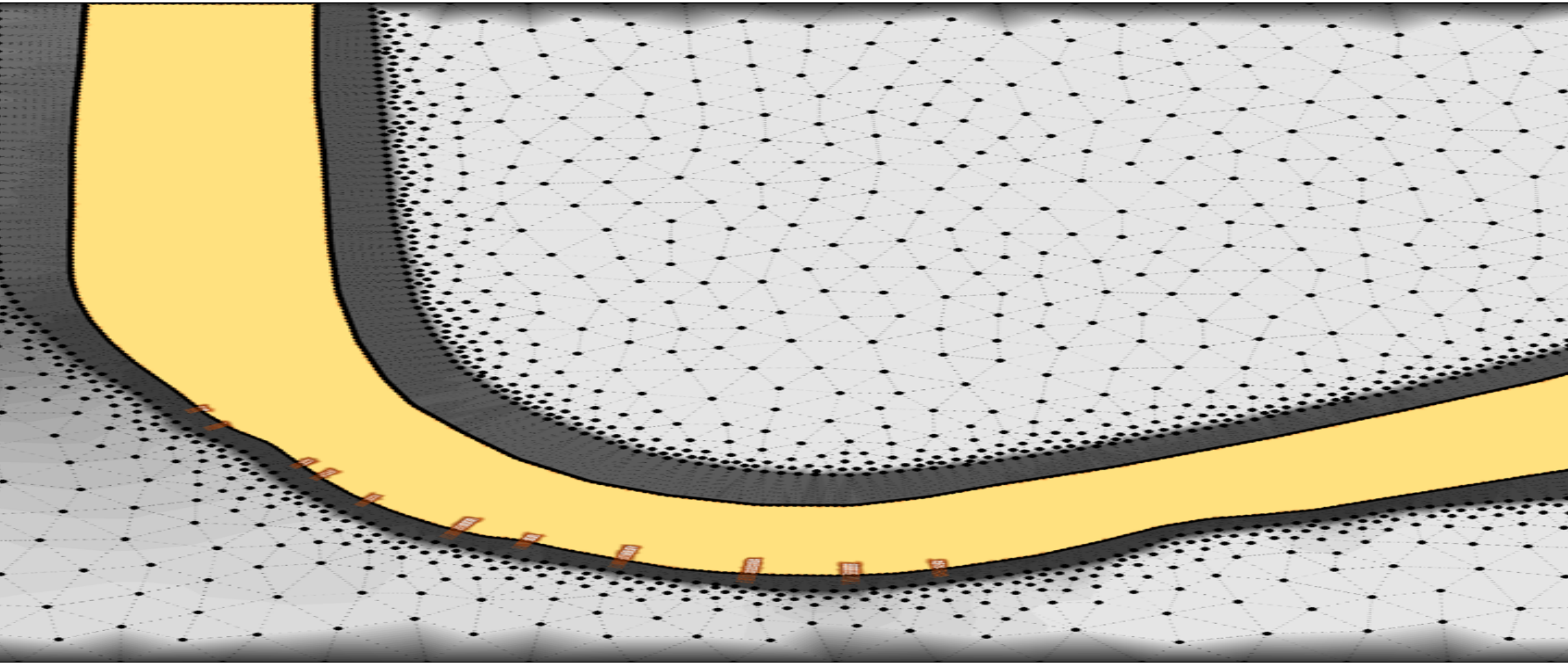
Simulation-based optimization of bank stabilization strategies



Vorticity magnitude at the surface

LES with grid resolution ~ 25 cm

Simulation-based optimization of bank stabilization strategies

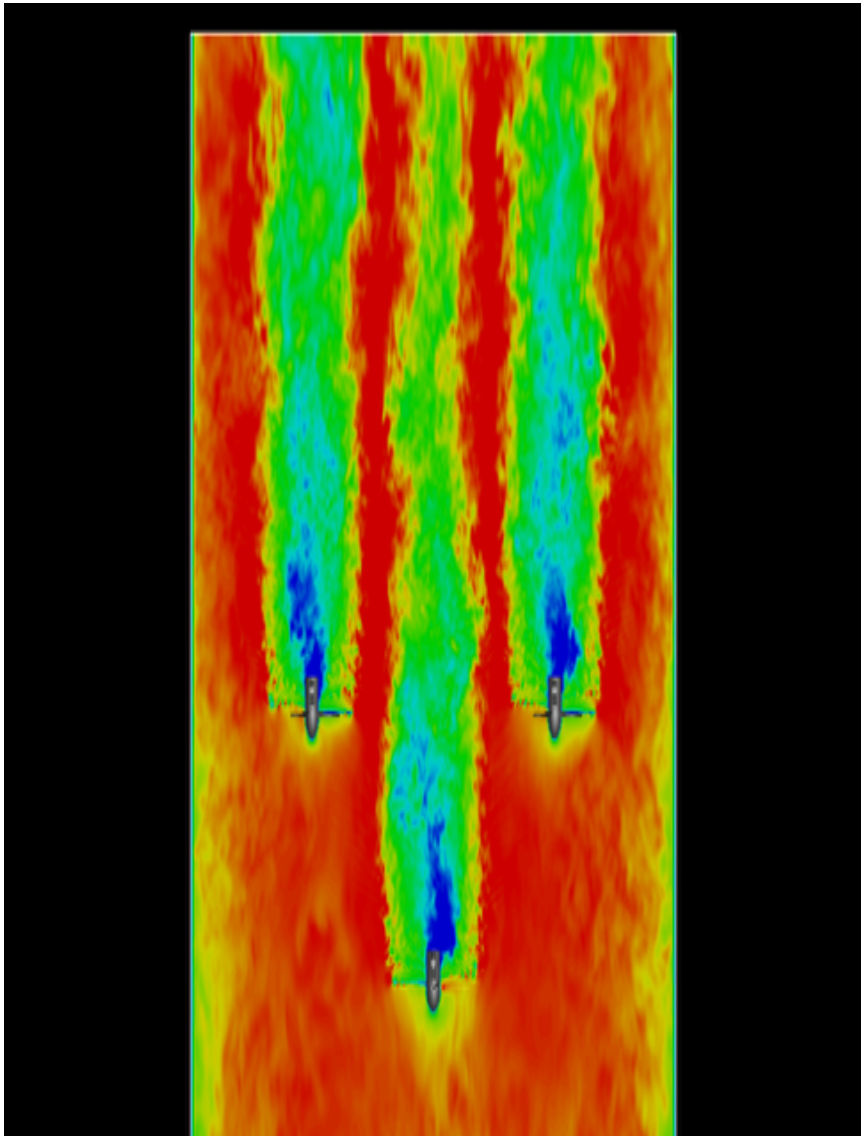


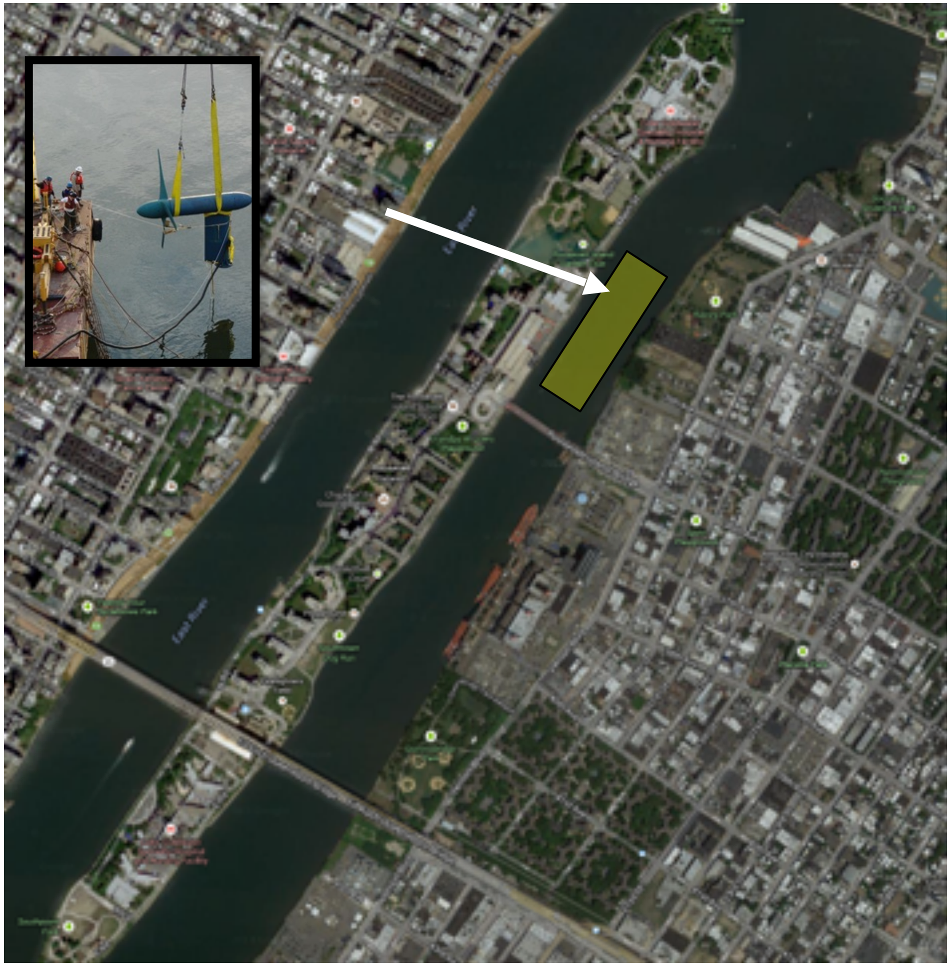
Morphodynamic evolution

29 days of physical time

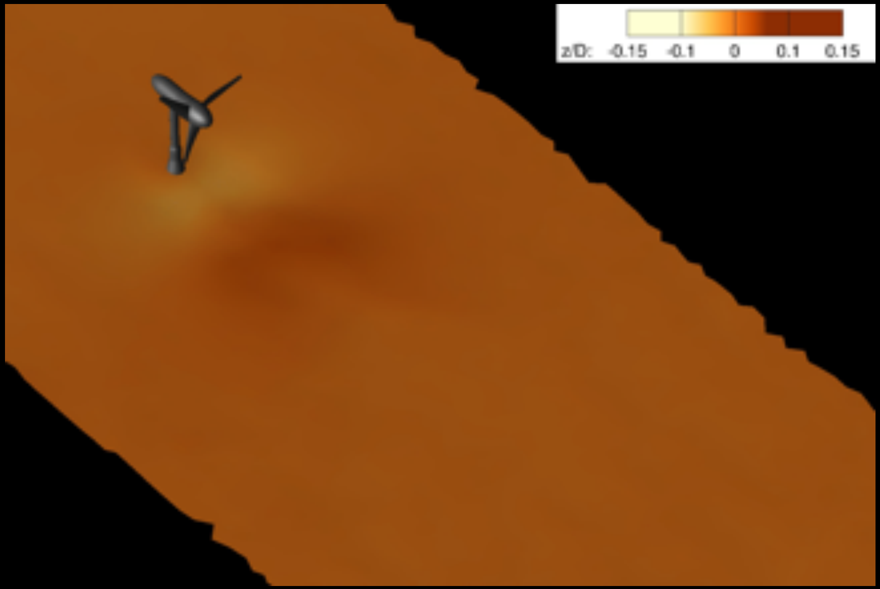
Simulation-based optimization of tidal energy resources

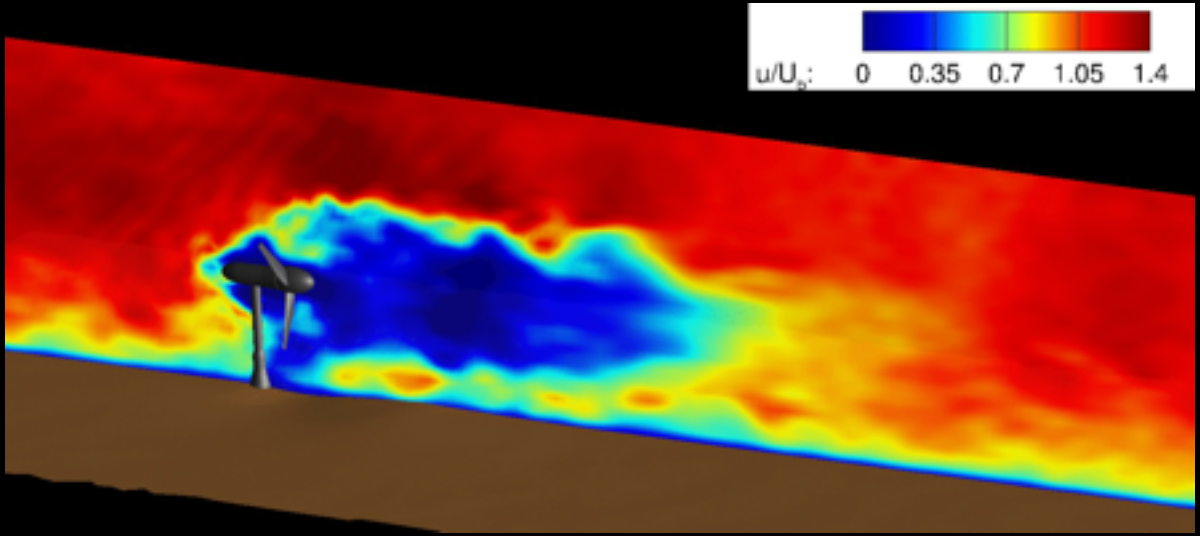
The Roosevelt Island Tidal Energy Project in NYC





Large-eddy simulation of turbine-flow-sediment interactions





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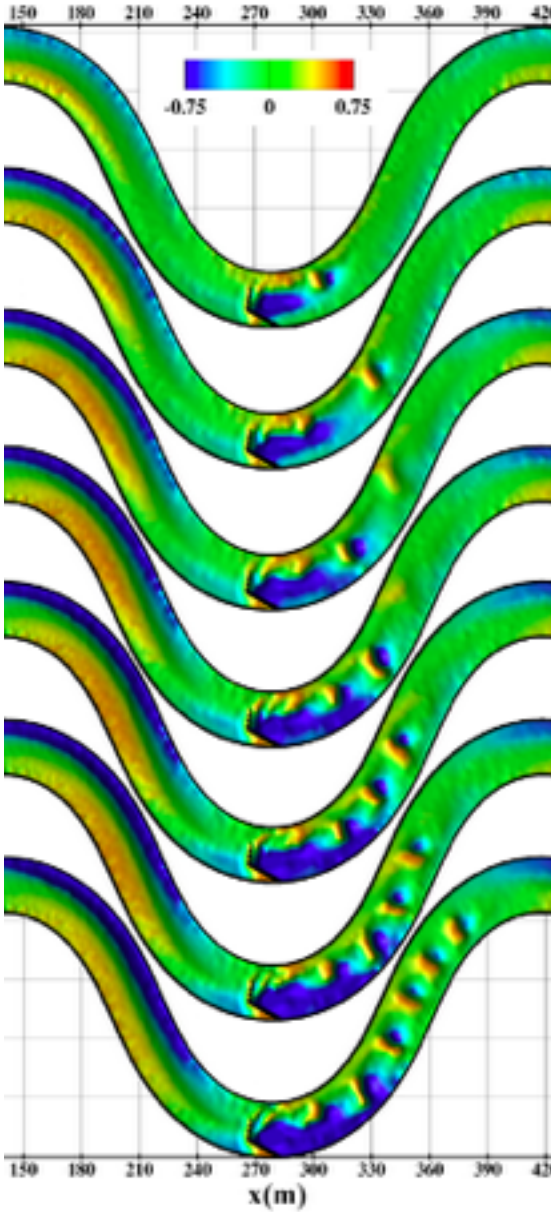

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