PetaScale Flow Simulations using Grids and Particles

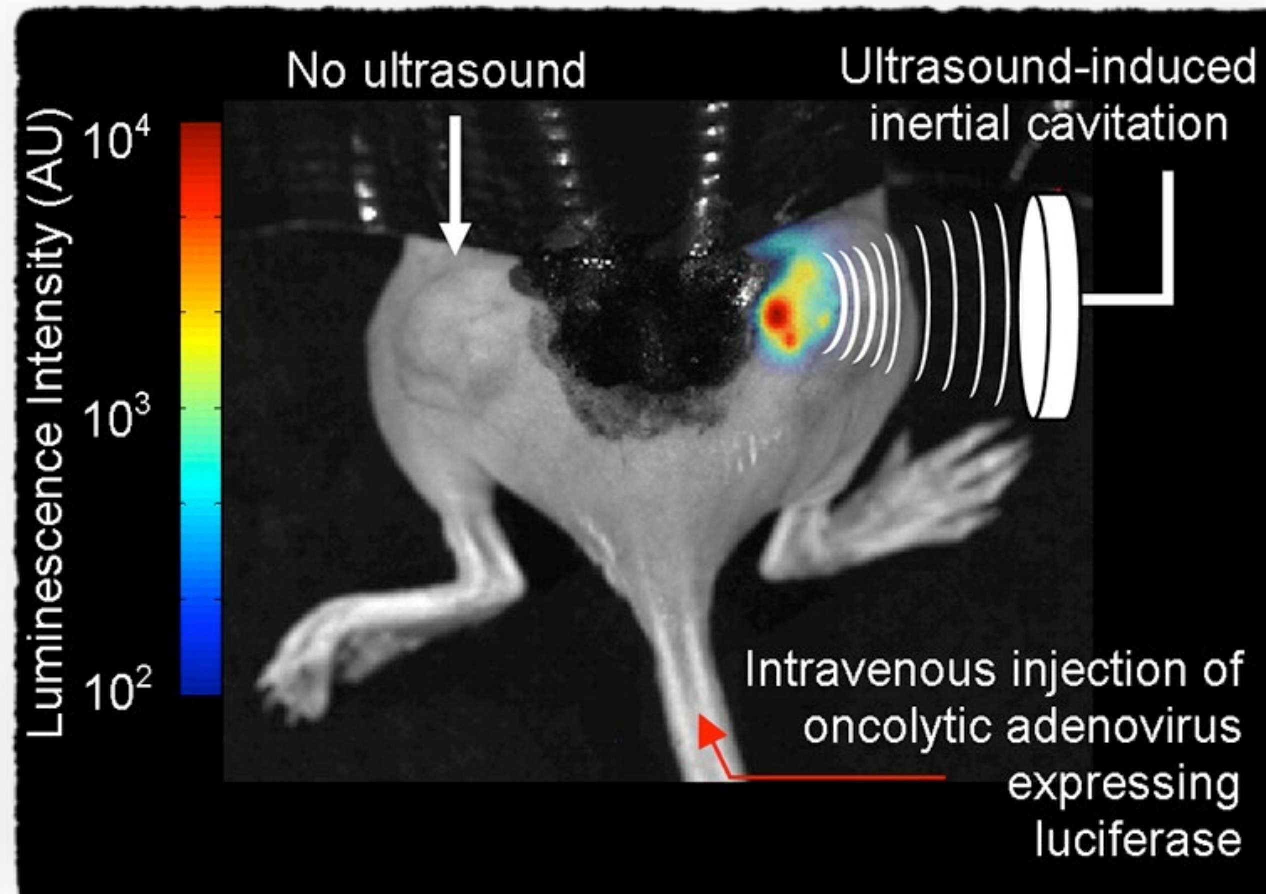
Petros Koumoutsakos

with: Diego Rossinelli, Babak Hejazialhosseini, Panos Hajidoukas,
Wim van Rees, Mattia Gazzola,
Jens Honore Walther, Michael Bergdorf

OUTLINE

- **WHY PETASCALE ?**
  - *when experiments and theory are not enough*
  - *for long time resolved simulations of fundamental flows*
  - *Inverse Design + Uncertainty Quantification for expensive models*
  - A KEY CHALLENGE: Computers and their effective implementation
- WHY GRIDS and PARTICLES?
  - Grids are Particles that do not move
  - Drastically different HPC implementation/performance
- **HOW TO STUDY FLUID MECHANICS OF COLLECTIVE PHENOMENA ?**
  - how to make fish to swim together - role of hydrodynamics

CAVITATION and DESTRUCTION

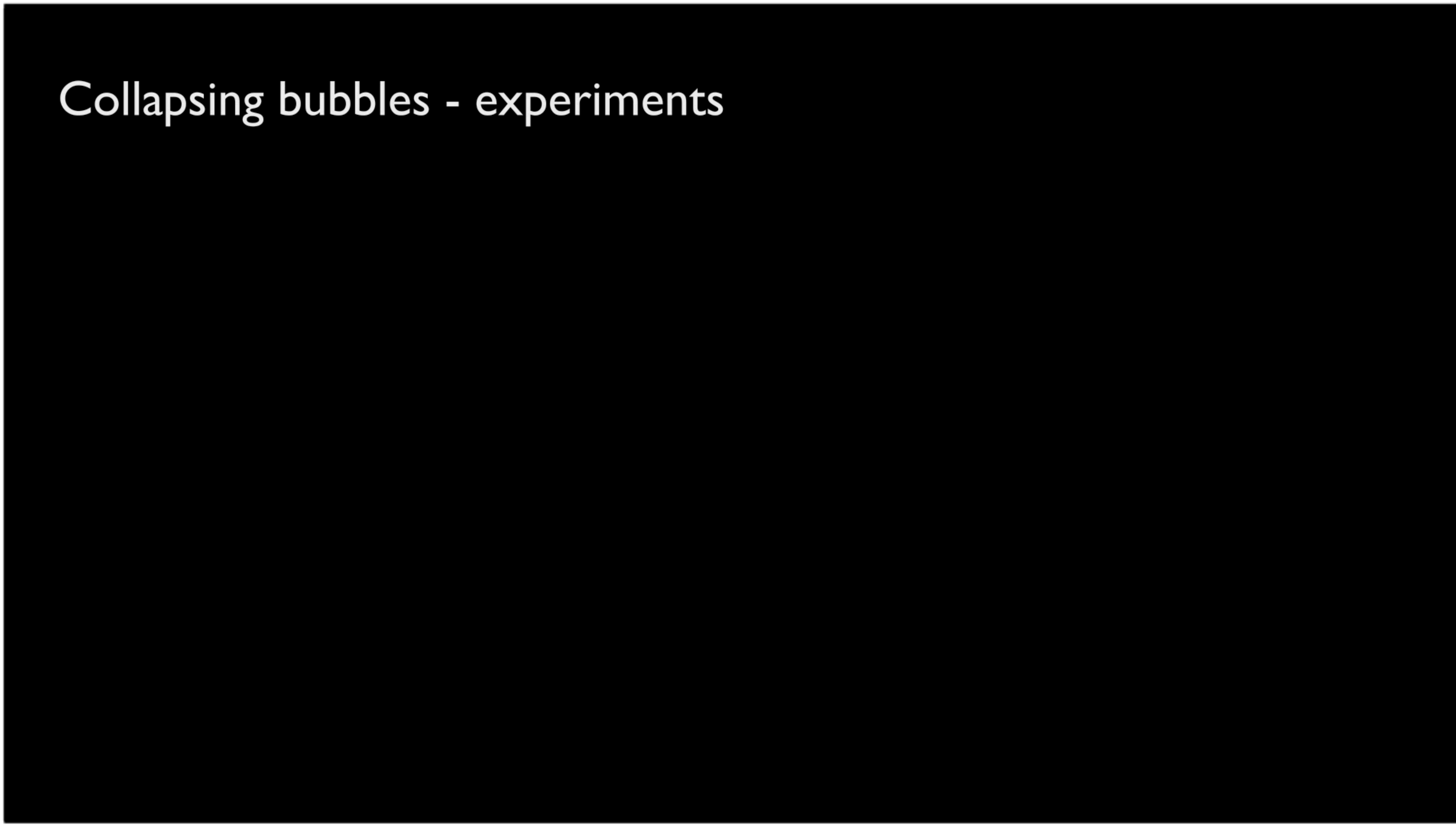


credit: C. Coussios Lab, Oxford U.

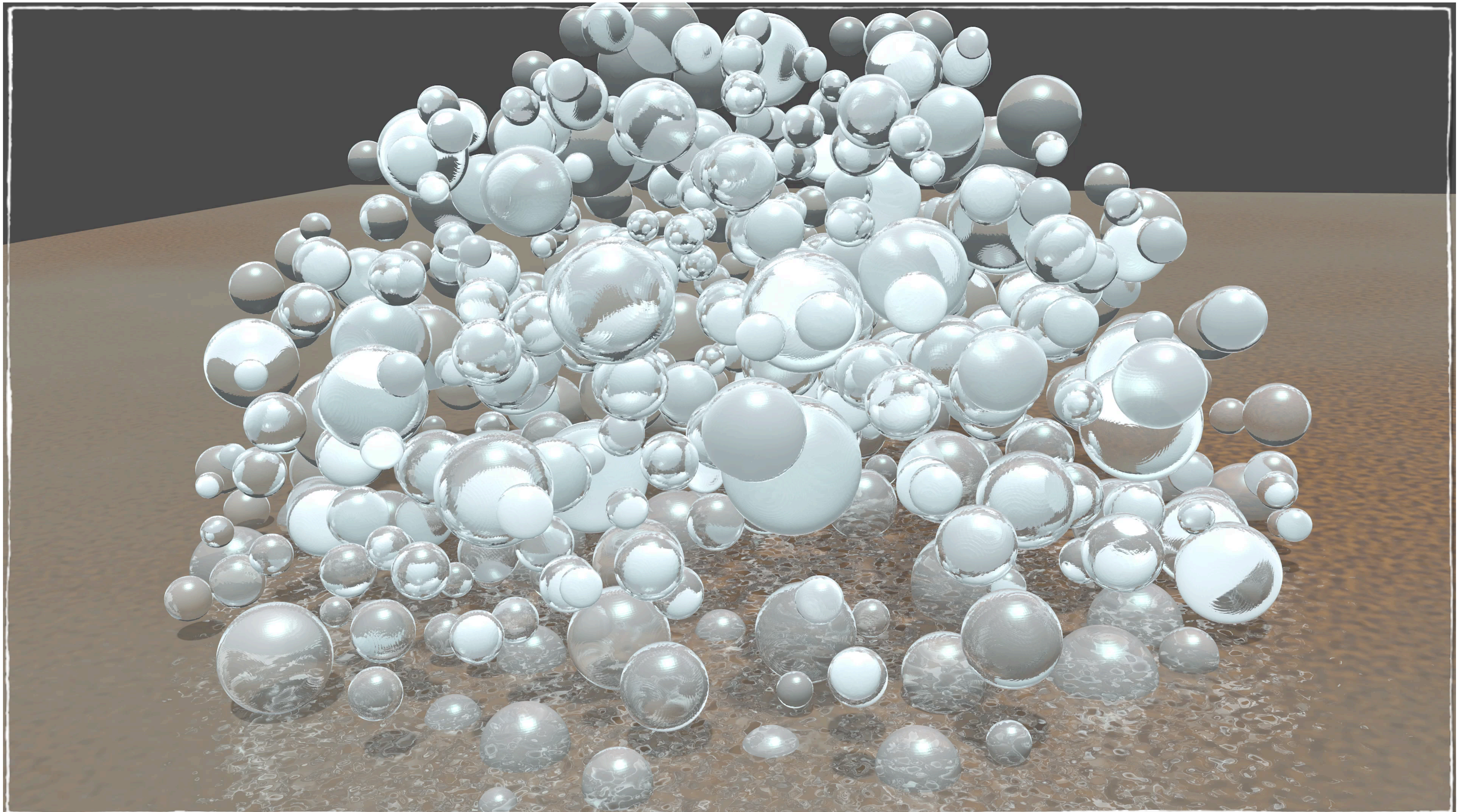
AVOID for Performance

HARNESS for Drug Delivery

CAVITATION – Experiments

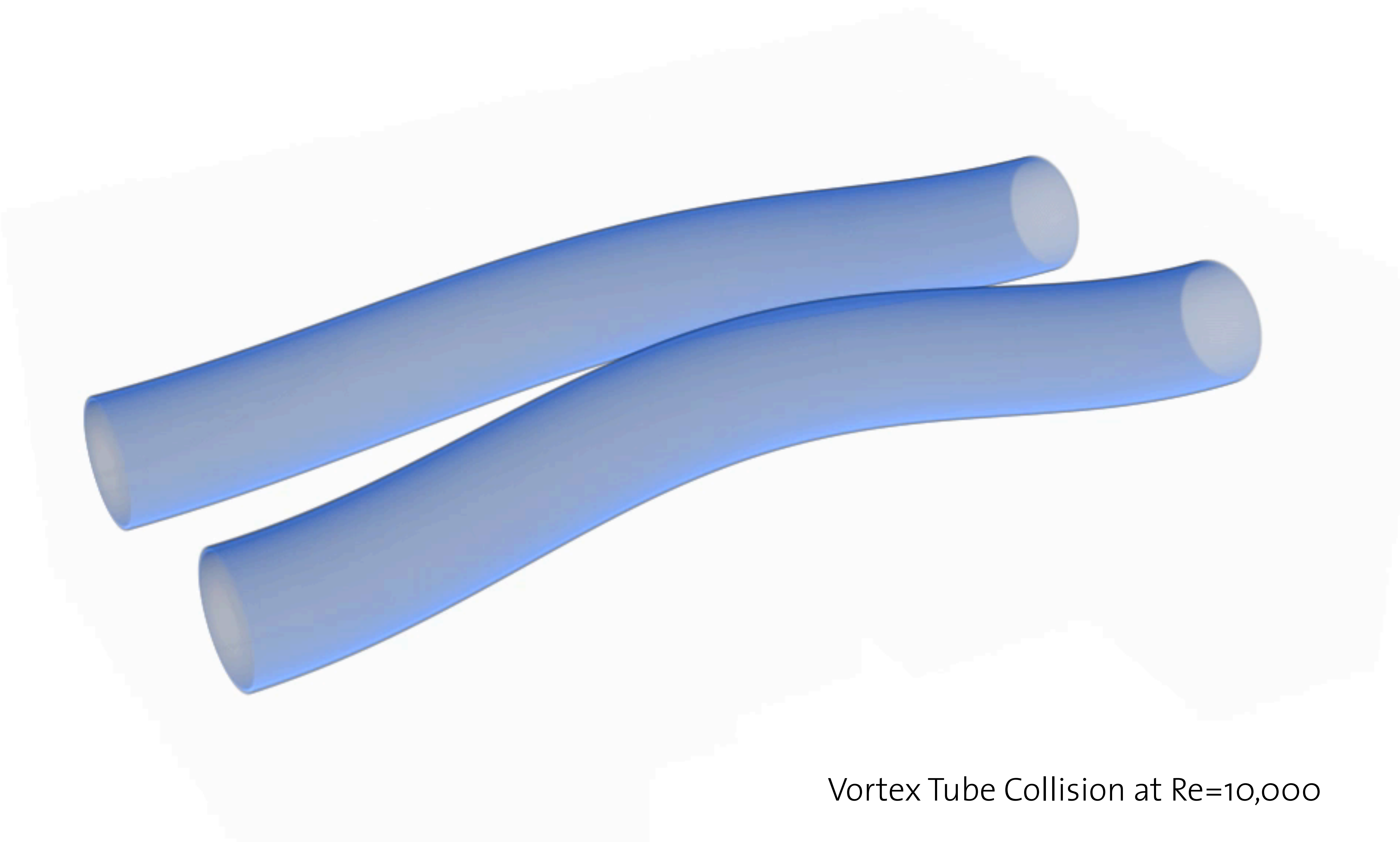


SIMULATIONS:Cloud Cavitation Collapse



(up to 15K bubbles)

...for long time resolved simulations of fundamental flows

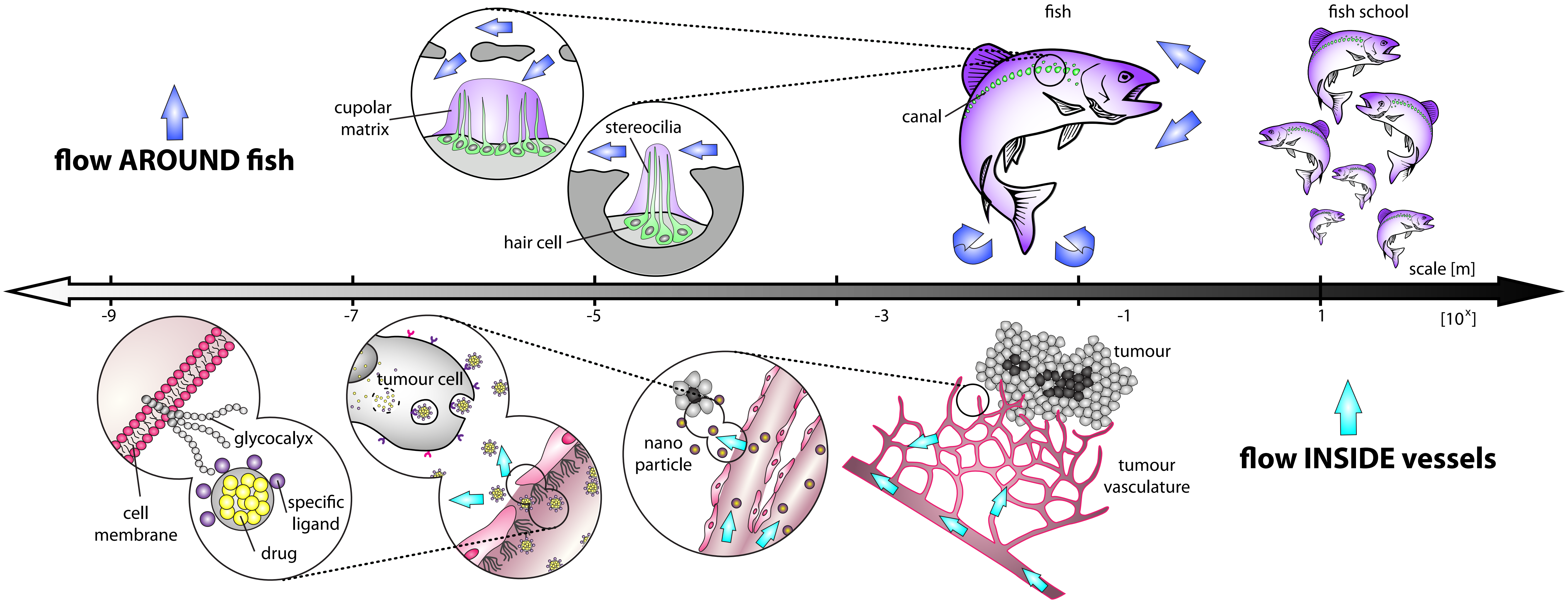


Vortex Tube Collision at Re=10,000

...inverse Design + Uncertainty Quantification for expensive models

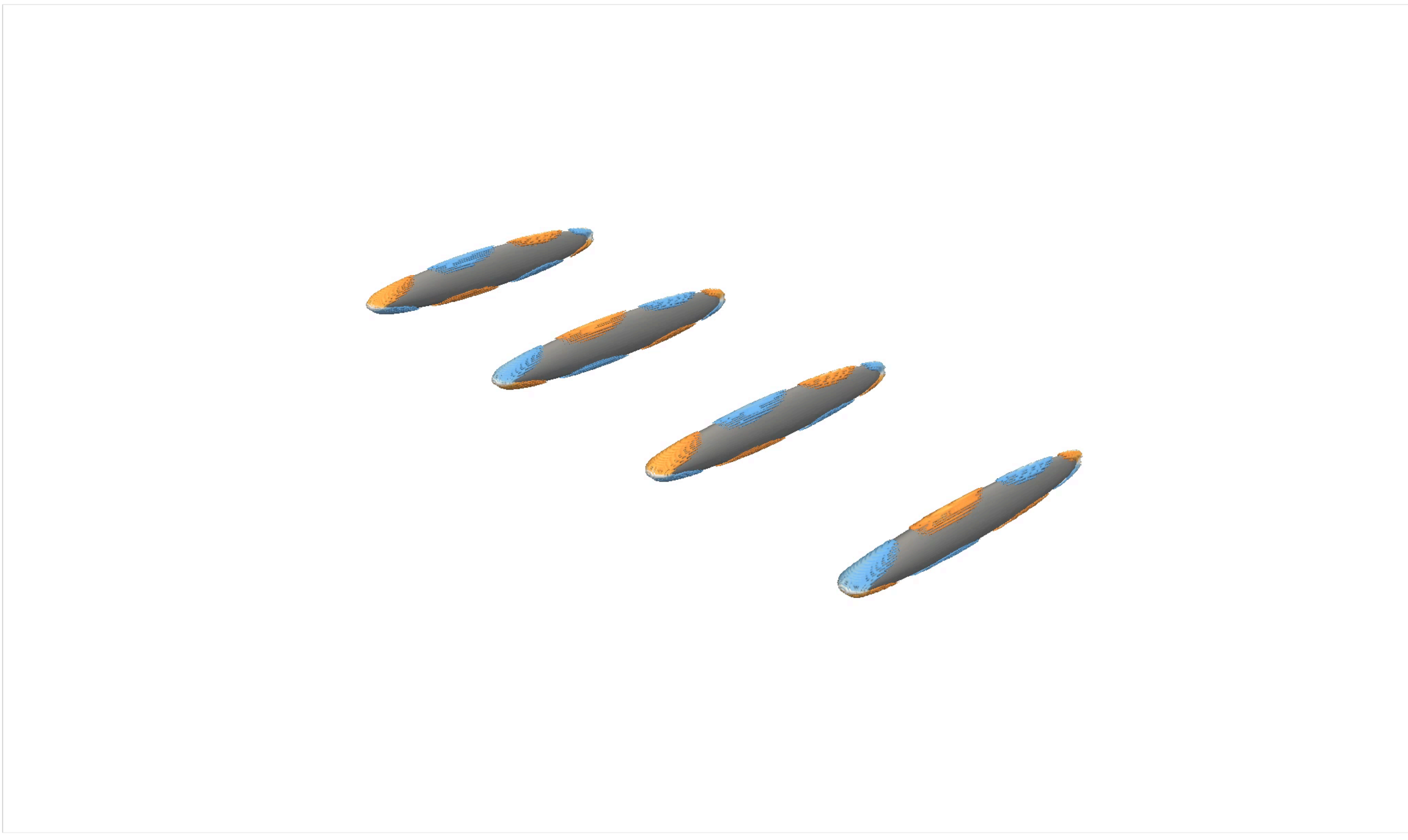
Hydrodynamics vs Behavior

Inverse Design + Uncertainty Quantification for expensive models

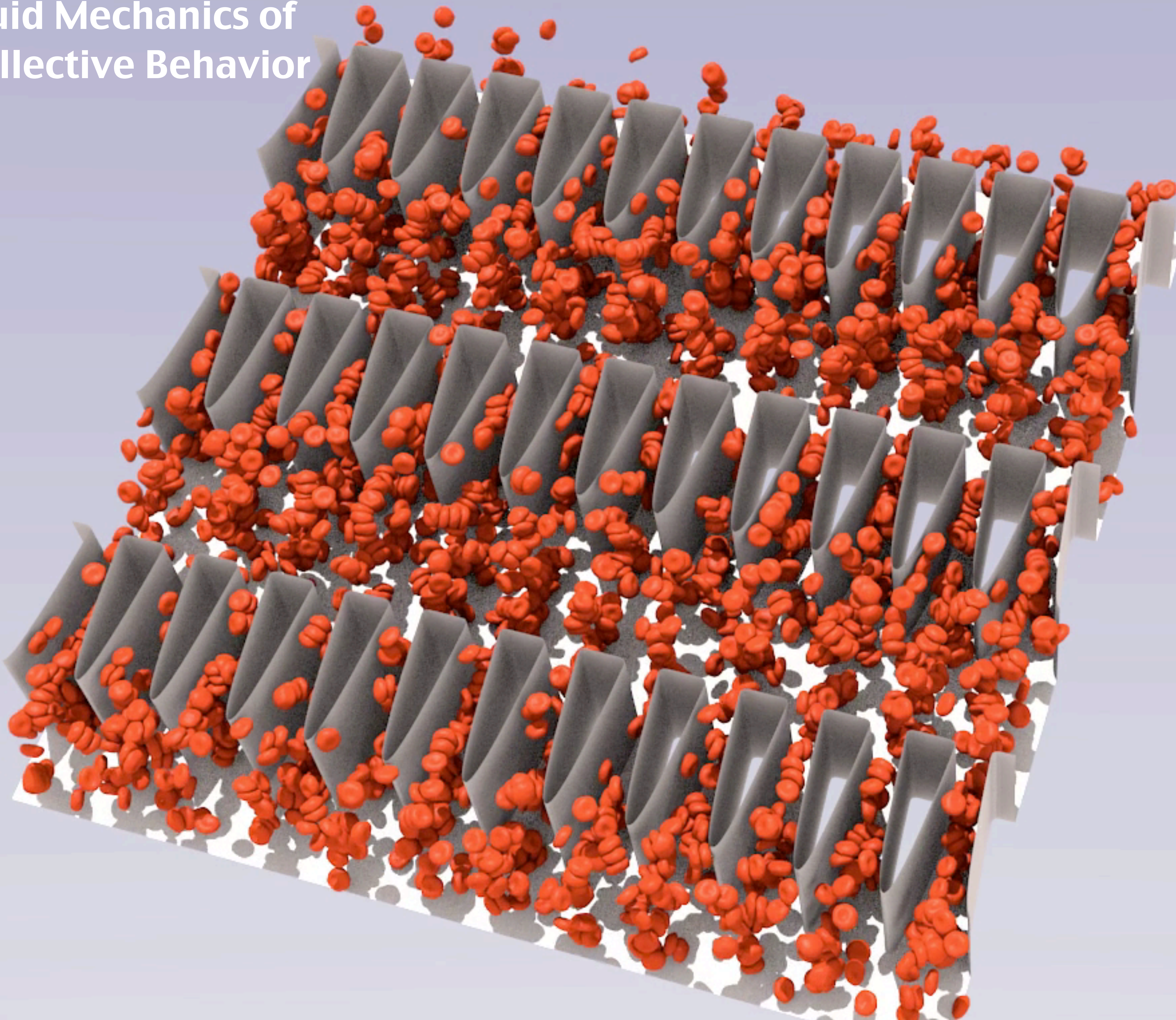


Fluid Mechanics of Collective Behavior

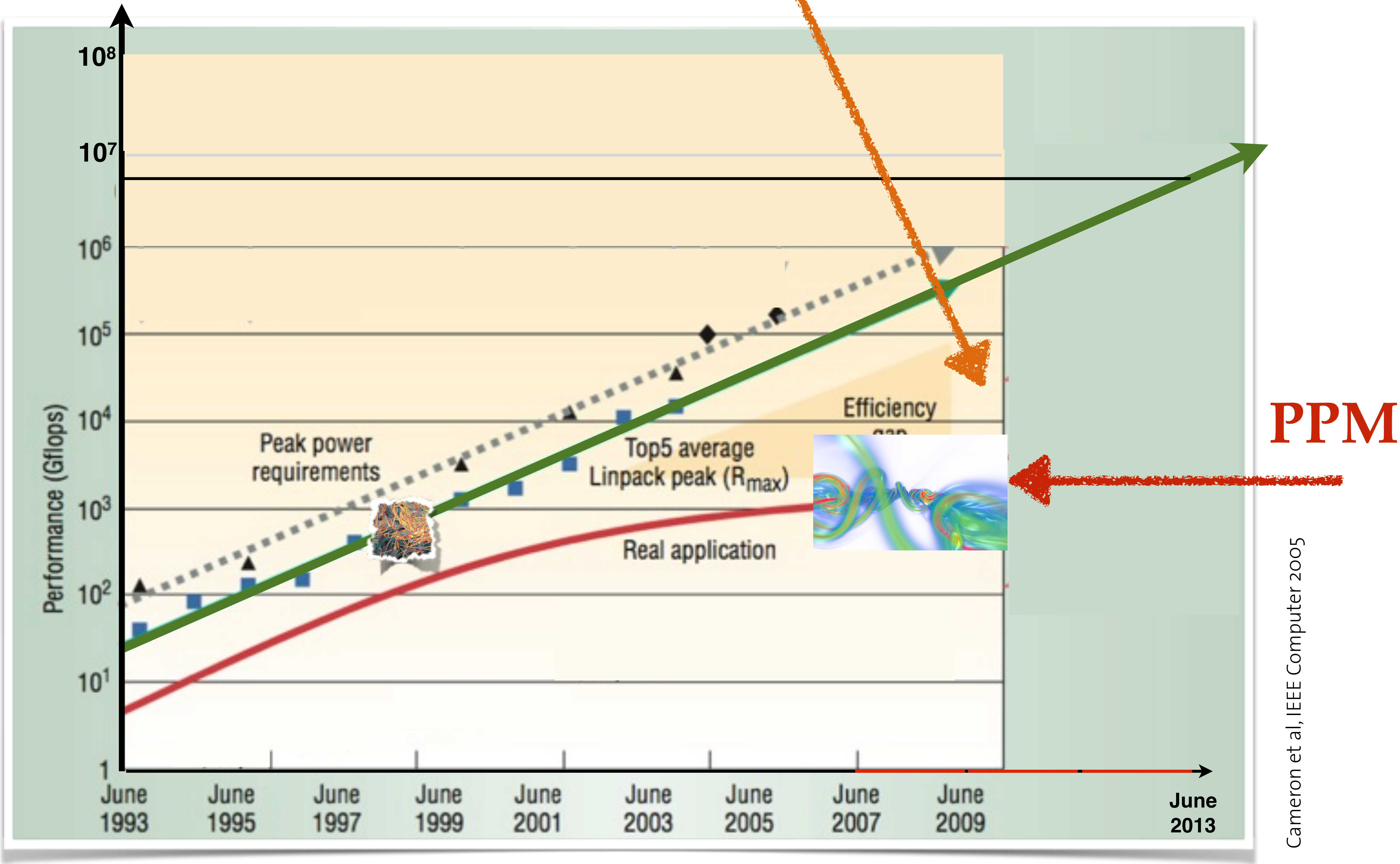
Fluid Mechanics of Collective Behavior



Fluid Mechanics of Collective Behavior



HPC and CFD: THE GAP

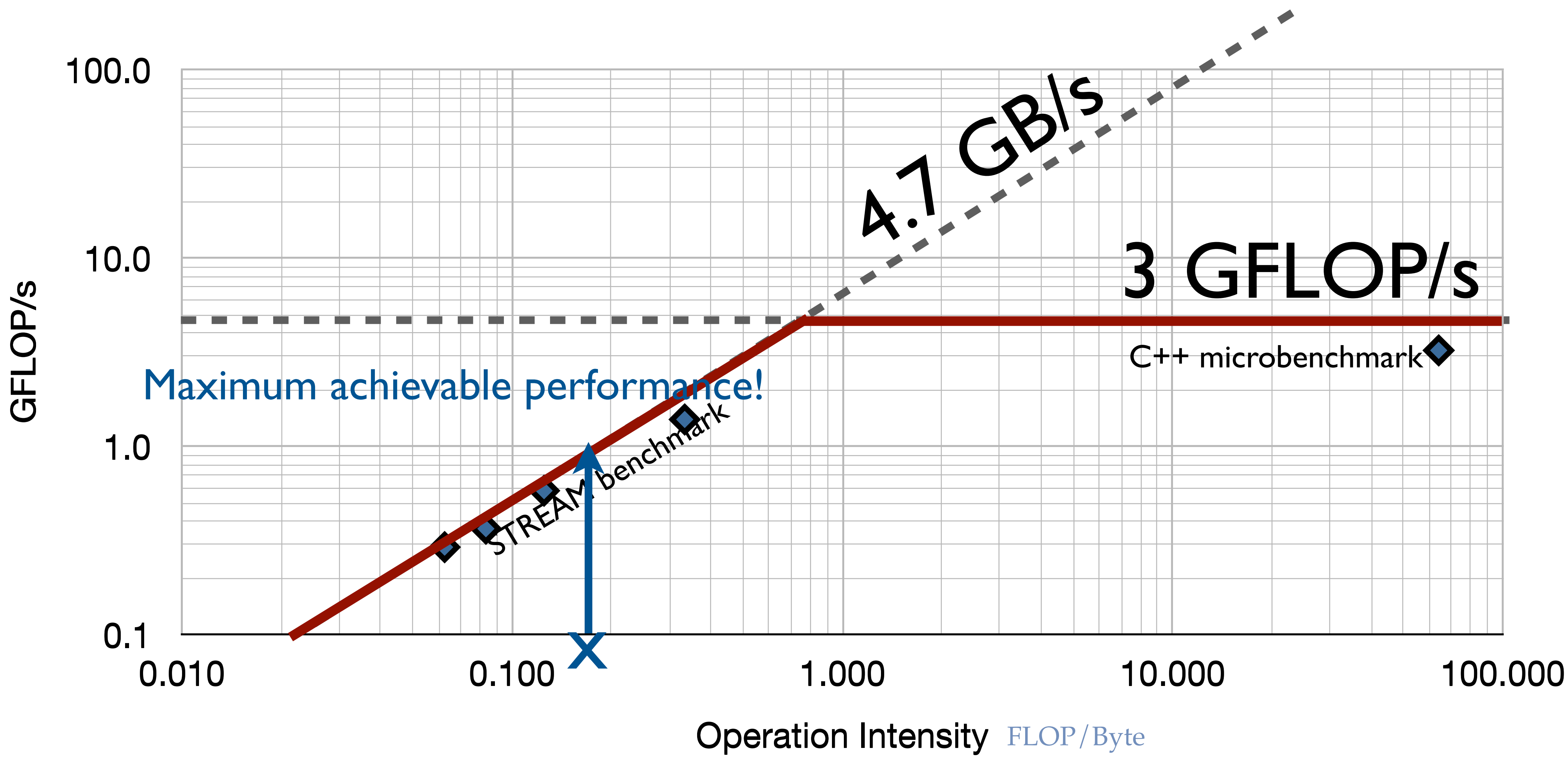


Cameron et al, IEEE Computer 2005

NOTE: **Chombo, Flash, Raptor, Uintah** < 10 % of the available performance

PERFORMANCE: Single Core & The Roofline Model

$$\frac{GFLOP}{sec} = \frac{GBytes}{sec} \times \frac{FLOP}{Byte}$$

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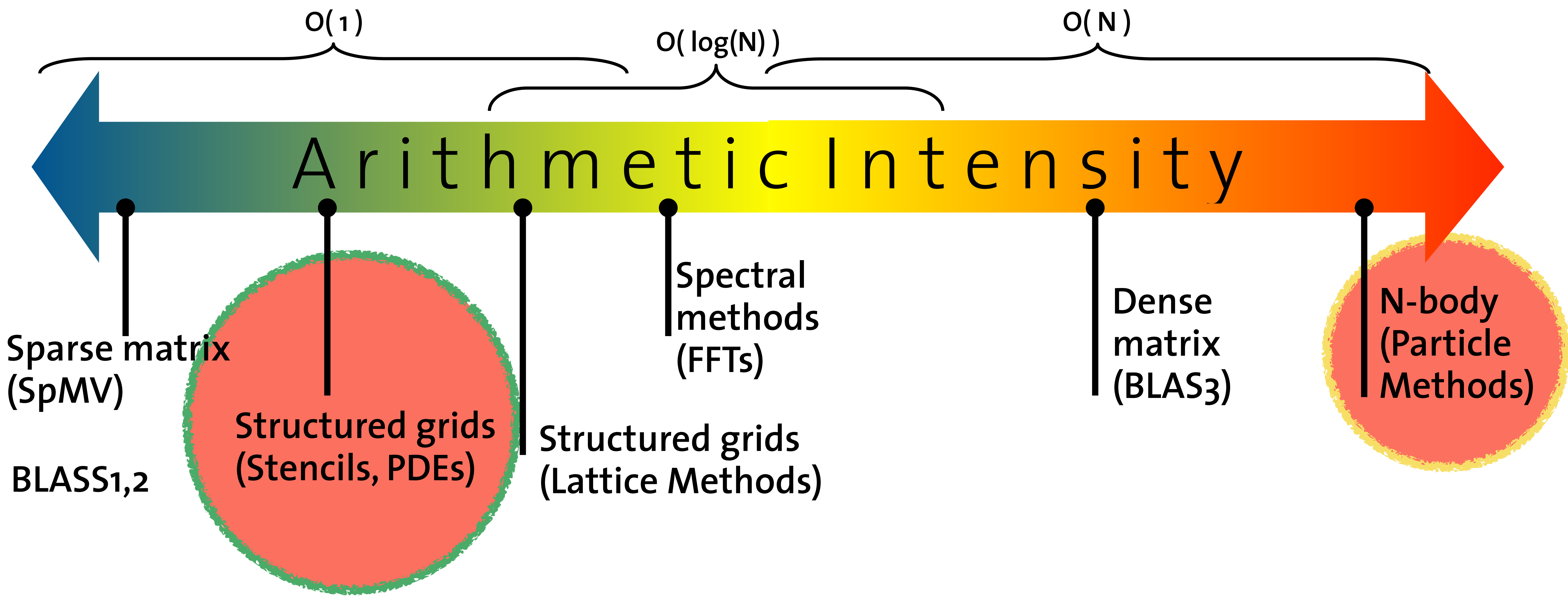
Example: a[i] = b[i]+ c[i]   % OI = 1/3
```

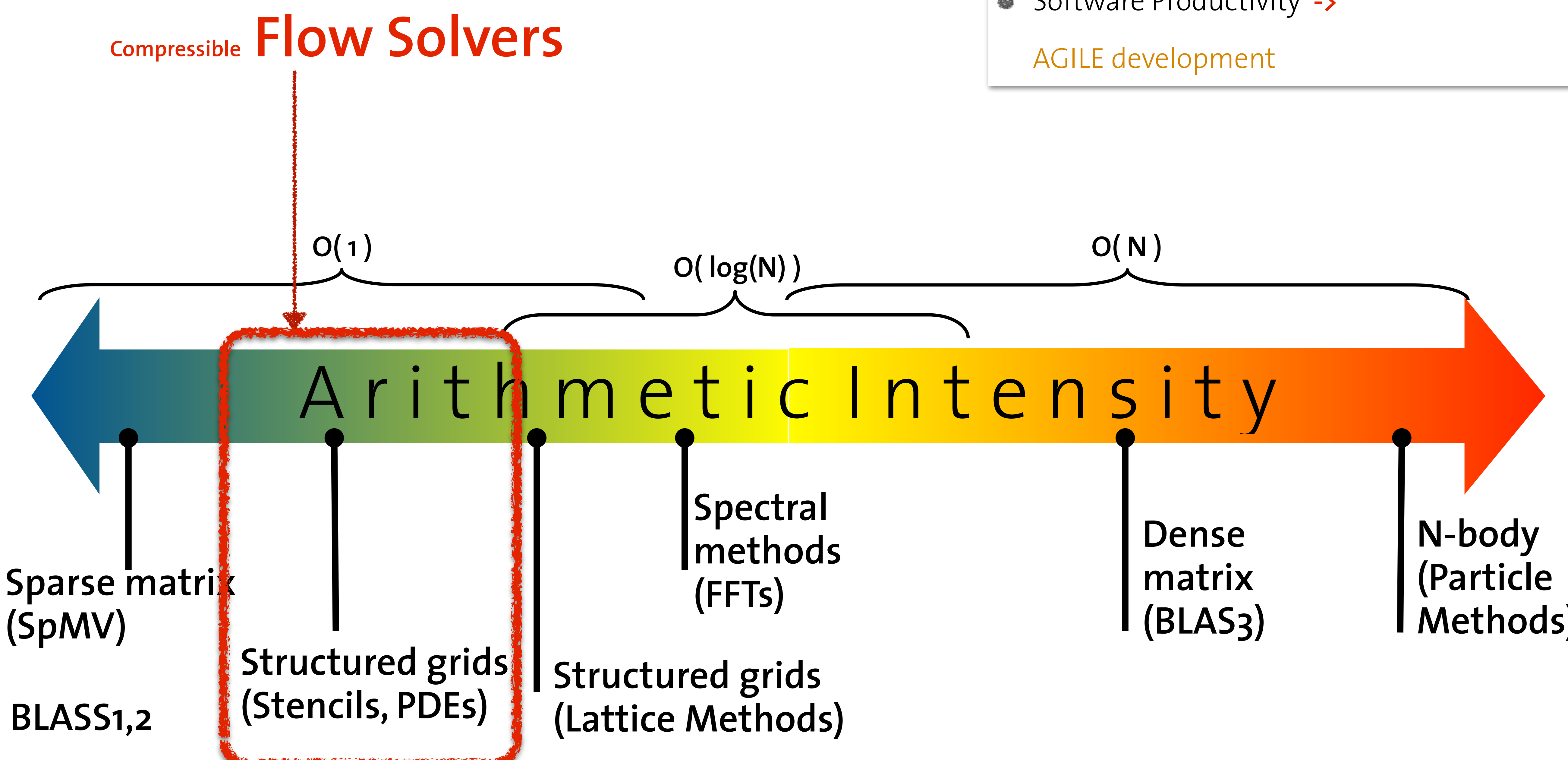
Roofline and the 7 Dwarfs



Computer Organization and Design, ***Patterson and Hennessy, MK Press, 2012***

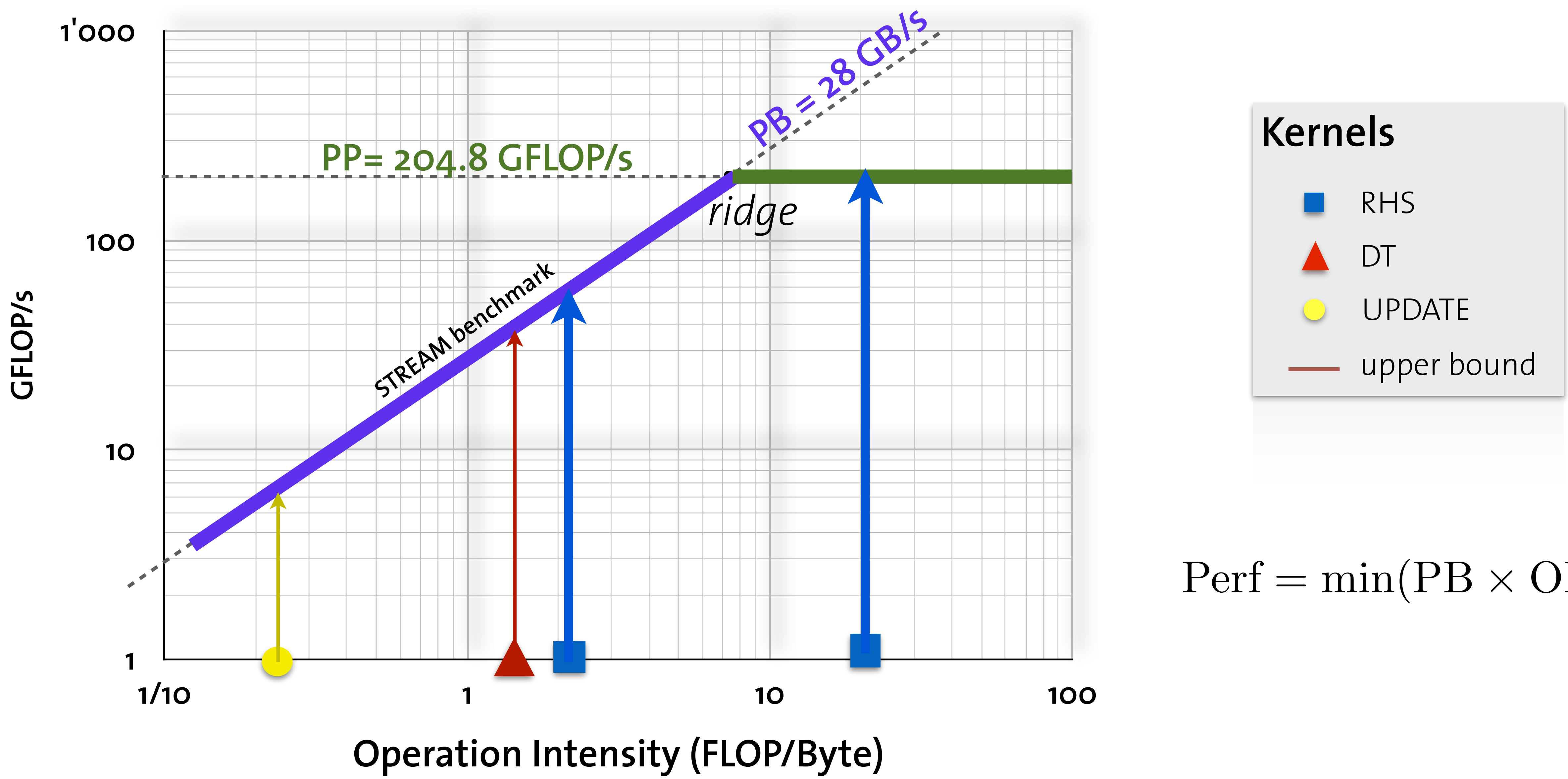
Roofline and the 7 Dwarfs

- Operational Intensity: Low FLOP/Byte ratios -> ALGORITHMS & DATA STRUCTURES
- FLOP/Instruction density -> ALGORITHMS & DATA STRUCTURES
- I/O Bandwidth and Storage Capacity -> wavelet COMPRESSION
- Software Productivity -> AGILE development



Computer Organization and Design, ***Patterson and Hennessy, MK Press, 2012***

Core/Node Performance: The Roofline of BG/Q



$$\text{Perf} = \min(\text{PB} \times \text{OI},\ \text{PP})$$

- **Operational Intensity:** FLOP count over off-chip memory transfer
- BG/Q **node** ridge point: (7.3 FLOP/Byte, 204.8 GFLOP/s)

PERFORMANCE/COMPARISONS

TIME TO SOLUTION (no I/O)

$$T_w = \Delta^{wt} * \frac{N_c}{N_p}$$

T_w = 1.8

T_w= 29.7 (TUM)

T_w= 16.3 - 39.0 (Stanford)

PFLOPS (% Peak)

14.4 PFLOPS (72%)

0.1 - 3% (TUM)

1.3 - 6.4% (2 racks - WENO) (Stanford)

MAXIMUM SIZE

1.3 E13 - 15K bubbles

1.2 E08 - 0.15K bubbles

0.4 E13 - Turbulence

I/O + Compression

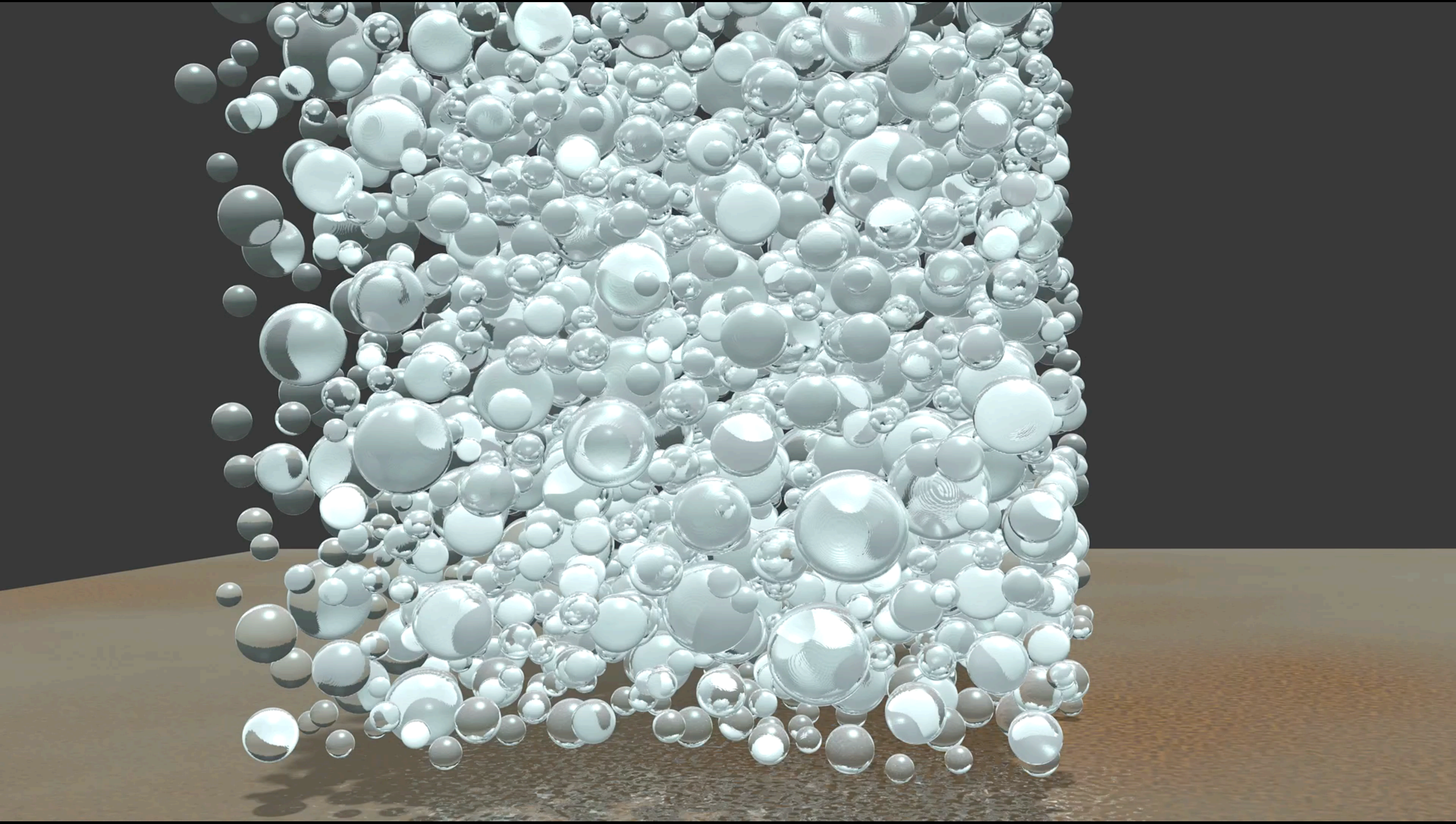
10X-100X

-

-

Sequoia supercomputer(LLNL) - 1.6M cores

Cloud Cavitation Collapse: β = 28



On Tue, Mar 10, 2015 at 11:33 AM, SC Support Team <sc@fz-juelich.de> wrote:
Dear JUQUEEN user,
yes indead, all our overtemperature events in March came from your application:

03.03.15 14:34:06 R02-M1-N06 F I 2322965 HWERR01 0004014D ::
This board was powered off due to **overtemperature**. : NodeTm2Reg=0xC0000000
05.03.15 15:32:29 R33-M1-N01 F I 2323670 HWERR01 0004014D ::
This board was powered off due to **overtemperature.** : NodeTm2Reg=0xC0000000
10.03.15 08:42:44 R02-M1-N06 F I 2323878 HWERR01 0004014D ::
This board was powered off due to **overtemperature.** : NodeTm2Reg=0xC0000000

2015-03-03 12:08:48 2015-03-03 14:35:03 146 pra0913 juqueen1c1.223921.0 2052448 LL15030312064874 R02-M1
8192 2954 - abnormal termination b
2015-03-05 15:04:53 2015-03-05 15:33:26 28 pra0913 juqueen1c1.225066.0 2056255 LL15030515030489 R33-M1
8192 3374 - END_JOB control action
2015-03-10 08:12:22 2015-03-10 08:43:42 31 pra0913 juqueen1c1.226134.0 2062798 LL15031008095035 R02-M1
8192 2878 - abnormal termination b

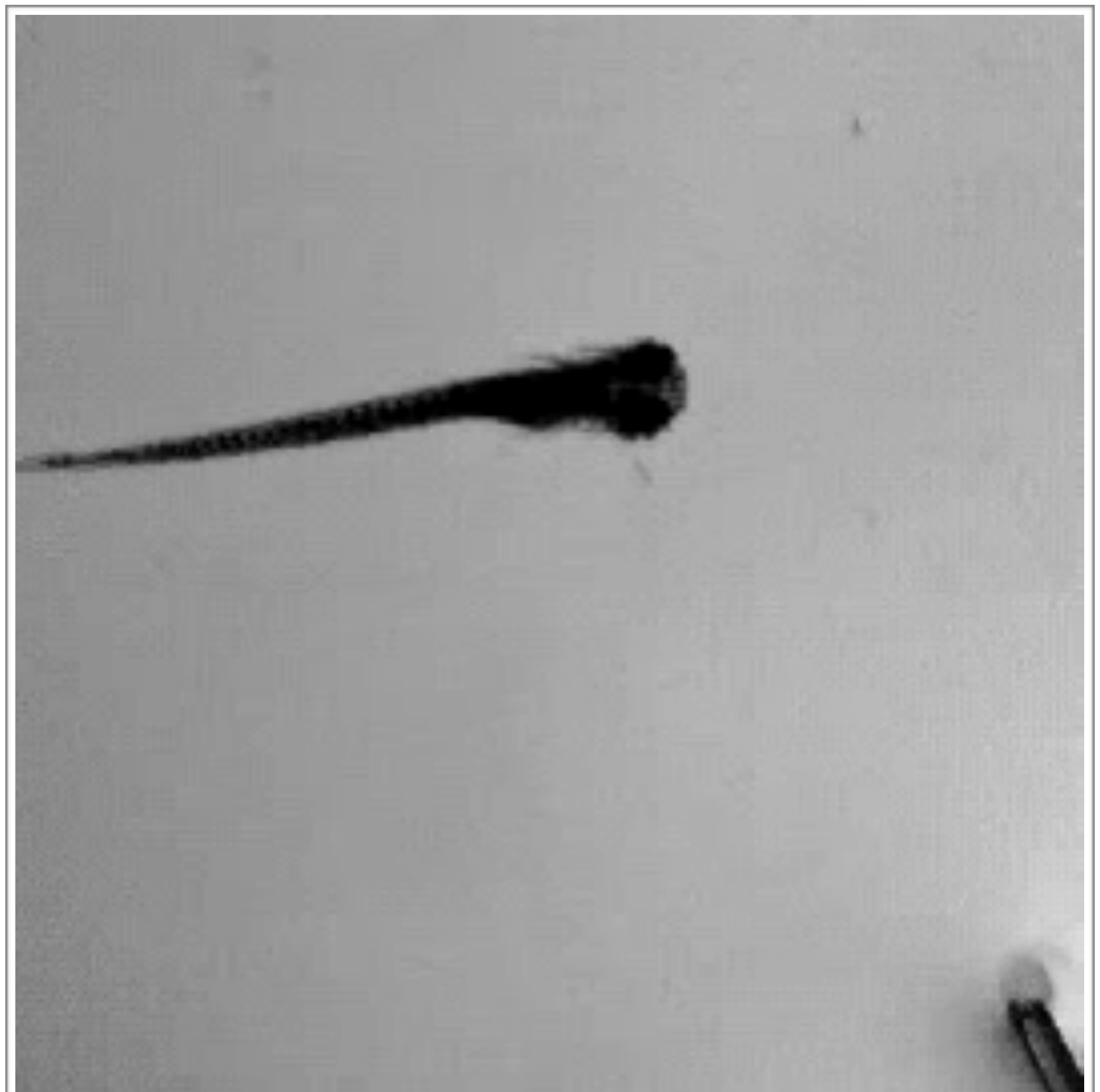
Nevertheless this is a hardware problem, where your program seems to put some stress on the node(board)s.
We have identified the nodes in question and worked on them, **including screwing down the cooling units, etc. and we are monitoring the temperatures more closely now.**

So please continue to resubmit the application and hopefully it will not run into that problem again.
Sorry for the inconveniences.
Jutta Docter

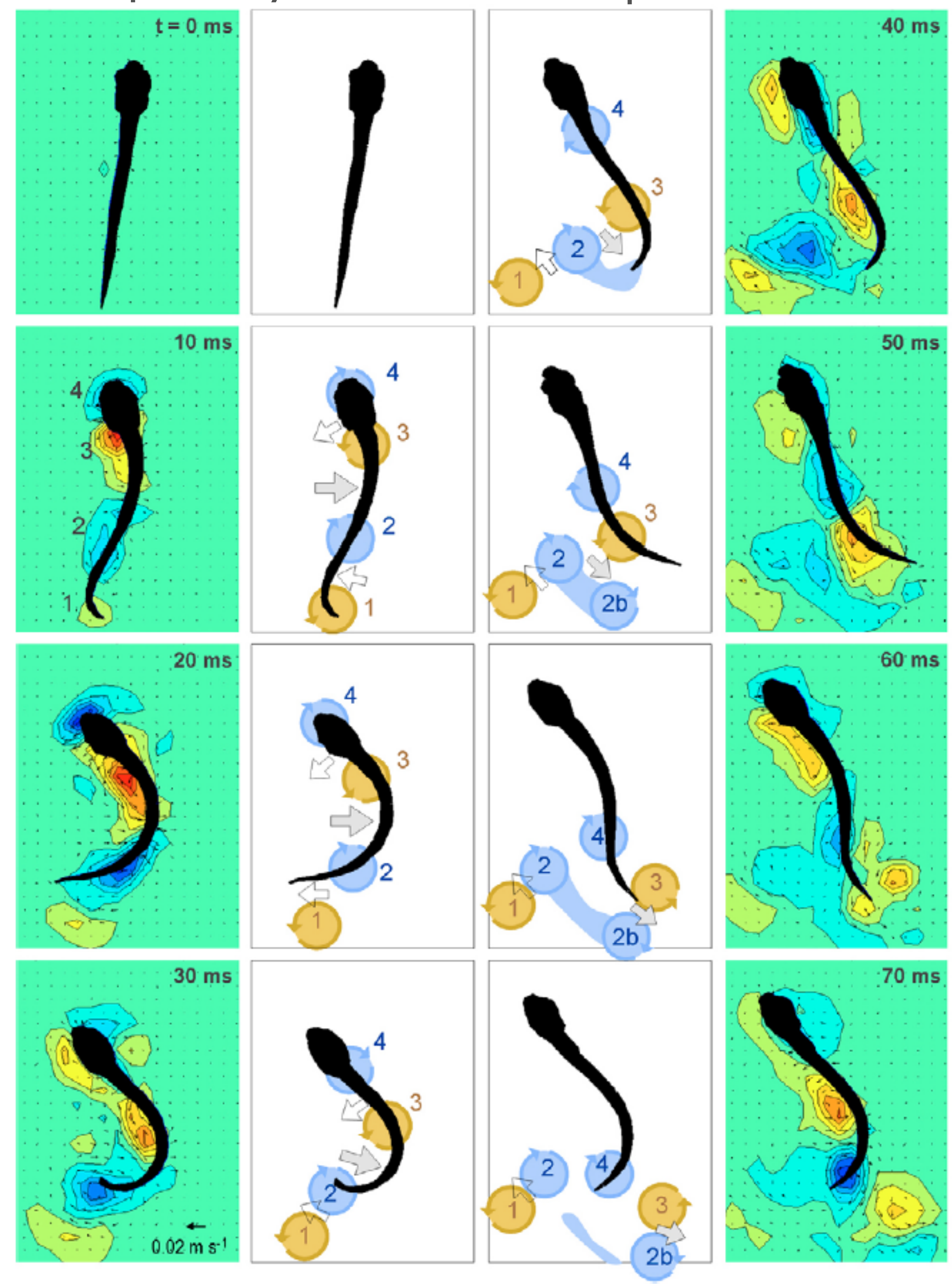
Videos Courtesy **Matt McHenry (UCI)** - *Zebrafish larvae evade predators by sensing water flow,* **J. Exp. Biol., 216, 2013**

C-start is an **escape** motion pattern

Is C-start **optimal?**



Liao Lab's Channel - YouTube

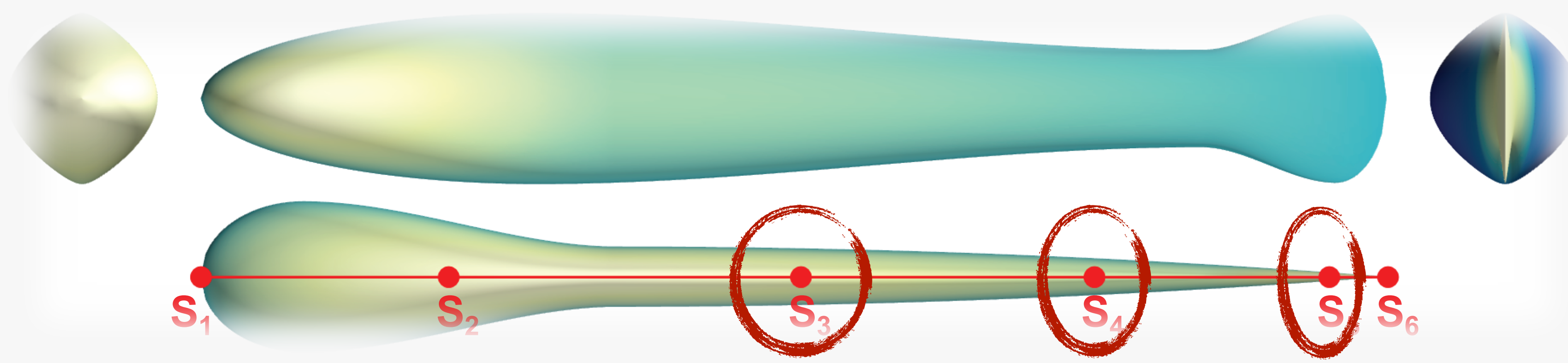


Muller, van den Boogaart, van Leeuwen. J. of Exp.Biology, 2008.

FLOW @ $Re = \frac{L^2/T_{\mathrm{prop}}}{\nu} = 550$

4.4mm long larva zebrafish of age 5 days post-fertilization

GEOMETRY



Muller, van den Boogaart, van Leeuwen. JEB, 2008
Parichy et al. Developmental Dynamics, 2009
Fontaine et al. JEB, 2008

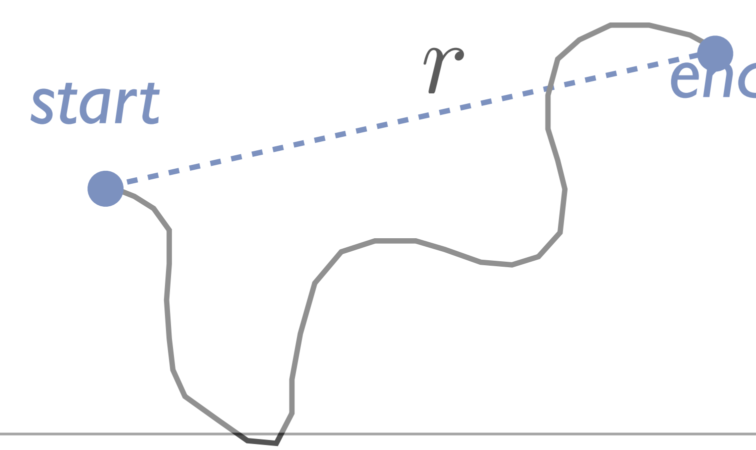
PARAMETERS

$$\kappa_s(s,t) = B(s)\, f\left(\frac{t}{T_{\mathrm{prep}} + T_{\mathrm{prop}}}\right) + K(s) \cdot \sin\left[2\pi\left(\frac{t}{T_{\mathrm{prop}}} - \tau(s)\right) + \phi\right]$$

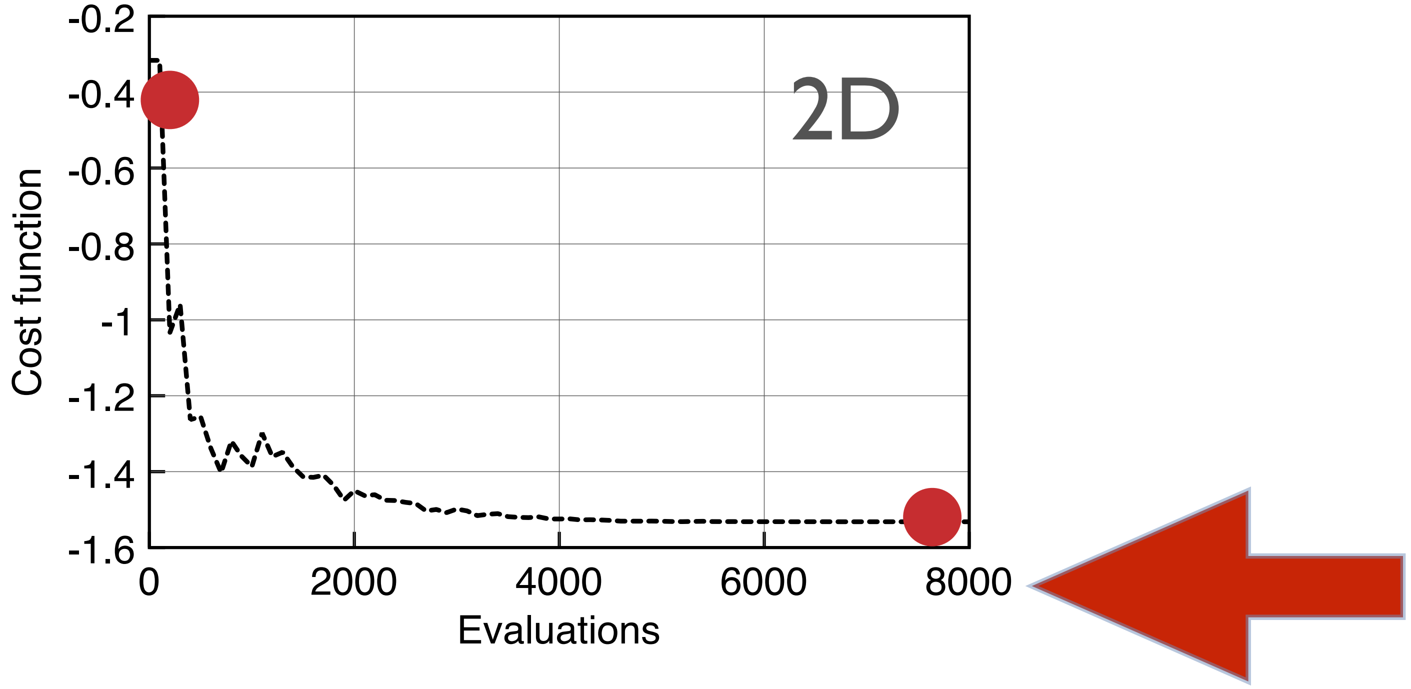
8 = 3 + 3 +1 +1

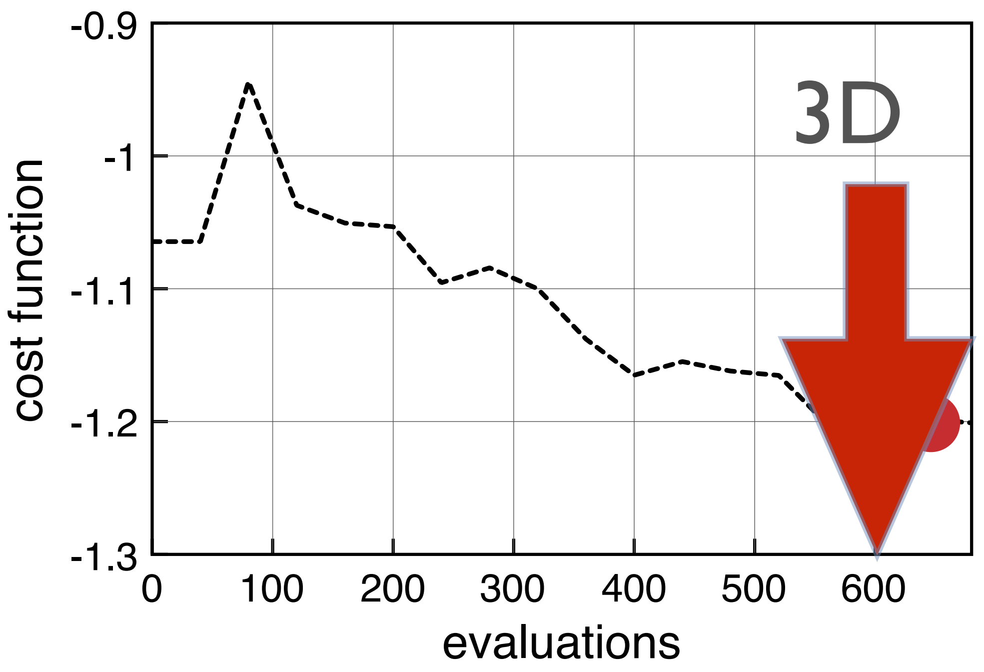
COST

$$f = -r\Big|_{T_{prep}+2T_{prop}}$$

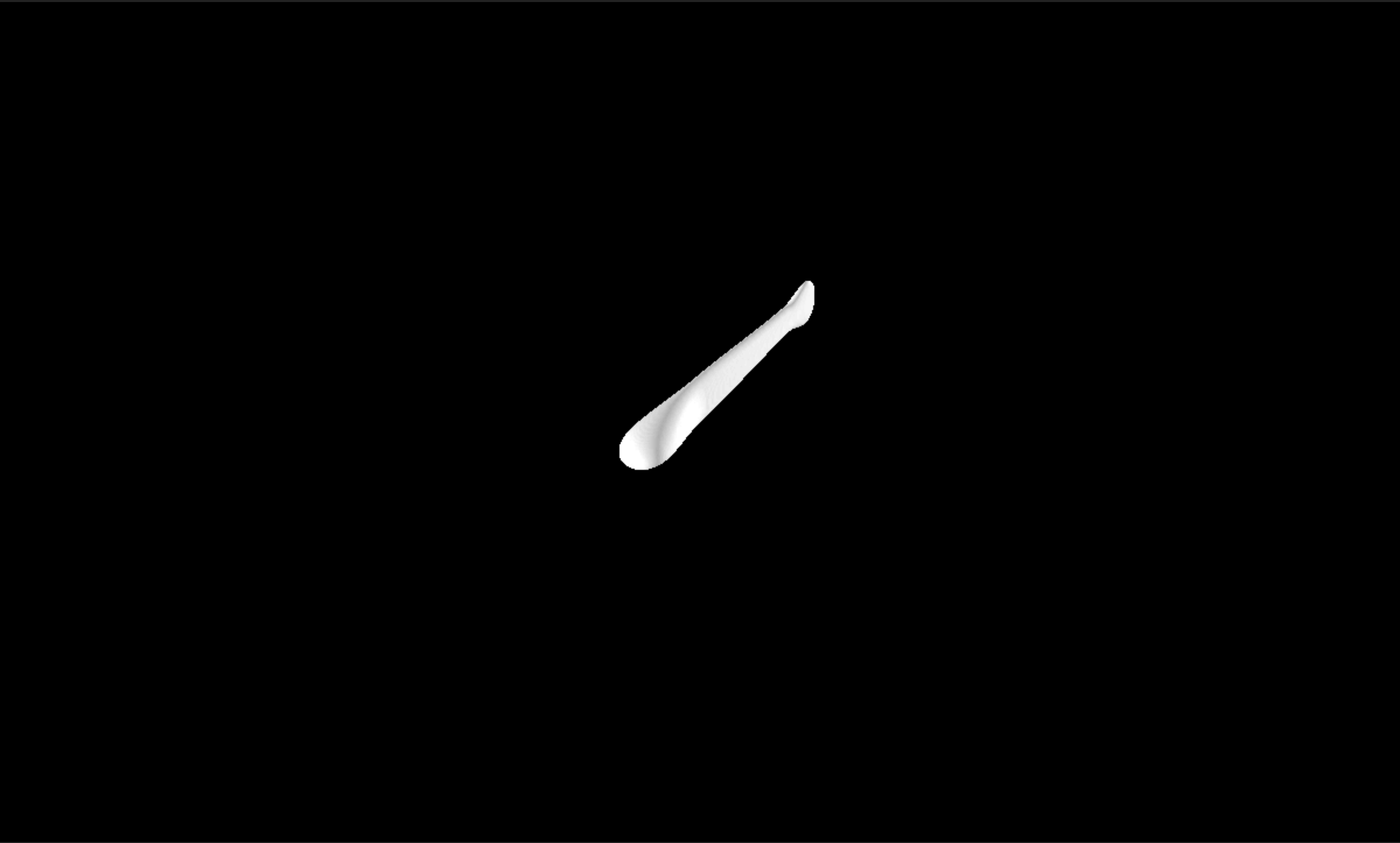


C-start is **OUTCOME** of optimization

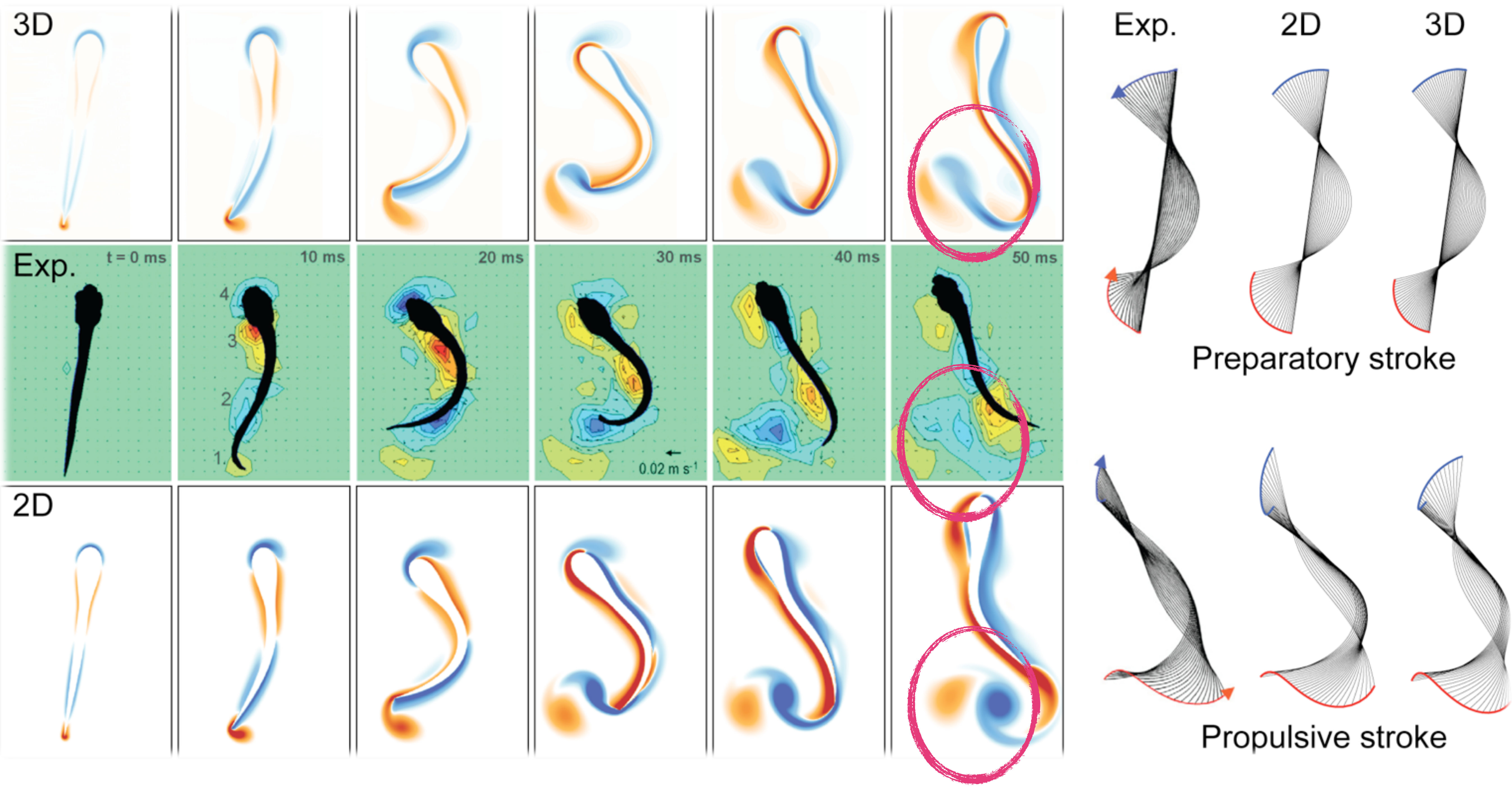




C-start: Vorticity Field

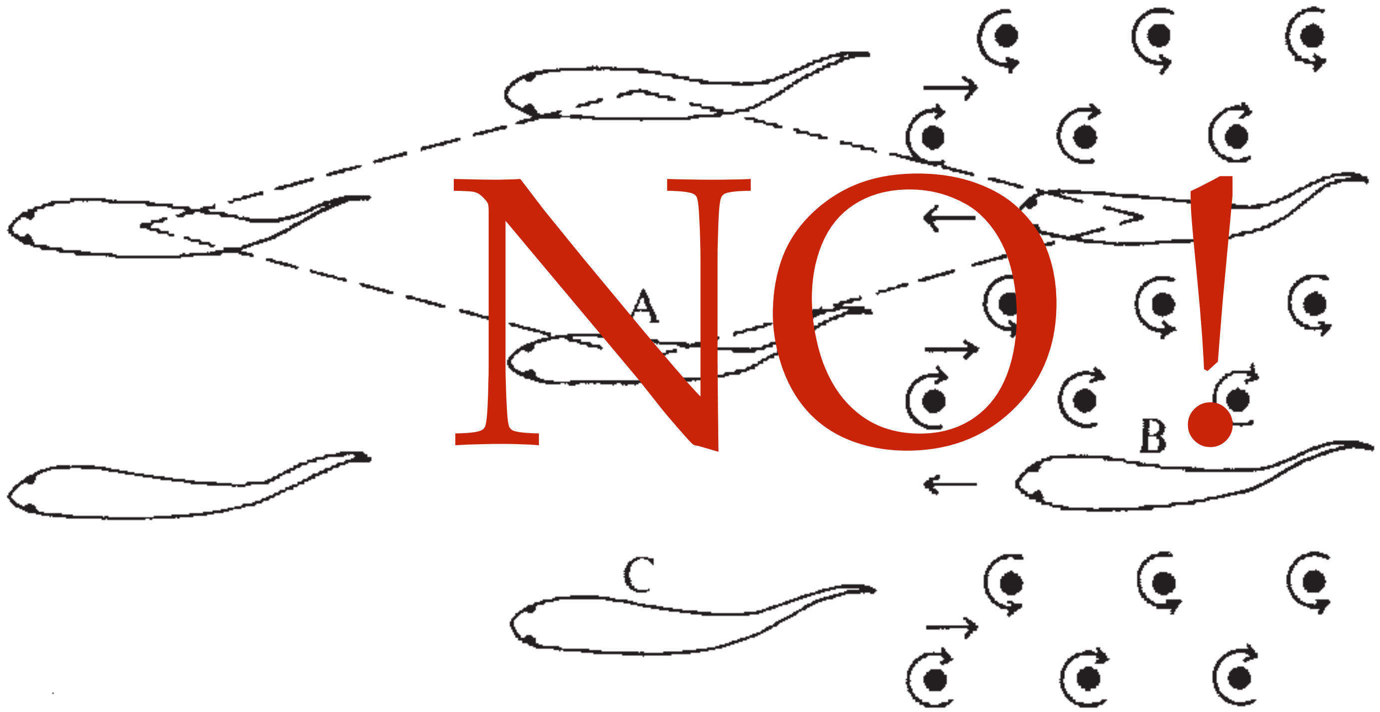


IN VIVO -*IN SILICO*



Experimental data by *Muller, van den Boogaart, van Leeuwen. JEB, 2008.*

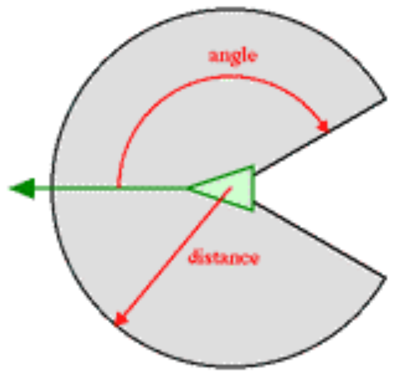
Schooling Hydromechanics



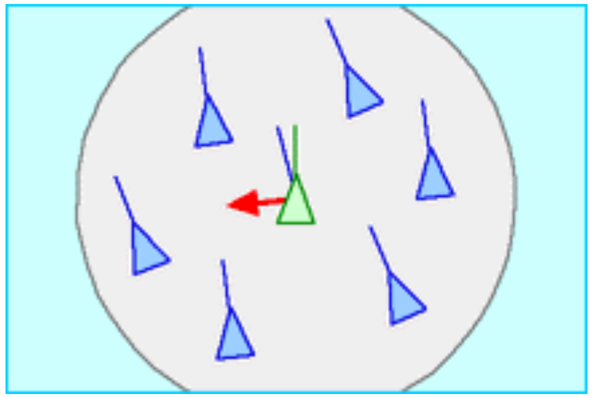
- **Diagnostic studies** used to investigate hydrodynamic benefits of schooling in structured formations
- **Rigid Formations:** Fish affect the flow but do not sense, respond, or take actions
- **Is there a benefit** of structured schooling from the hydrodynamic standpoint ?

[1] D. Weihs. Hydromechanics of fish schooling. Nature, 241(5387):290–291, 1973.
[2] J. Zhang, S. Childress, A. Libchaber, and M. Shelley. Flexible filaments in a flowing soap film as a model for one-dimensional flags in a two-dimensional wind. Nature, 408:835–839, 2000.

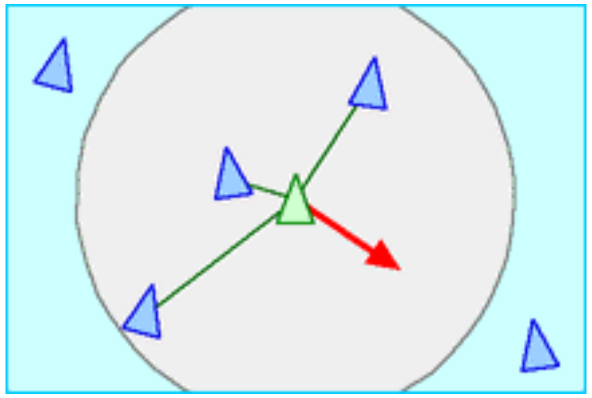
Swarm : 3 basic Rules for Steering an Agent



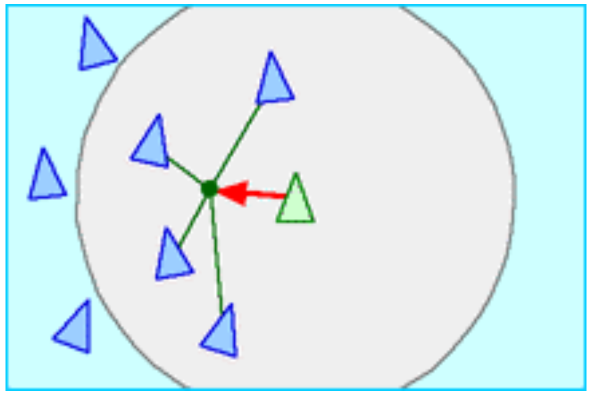
ALIGNMENT: towards the **local heading** of the mates



SEPARATION: **avoid crowding** mates



COHESION: towards the **average position of local** mates



http://www.red3d.com/cwr/boids/

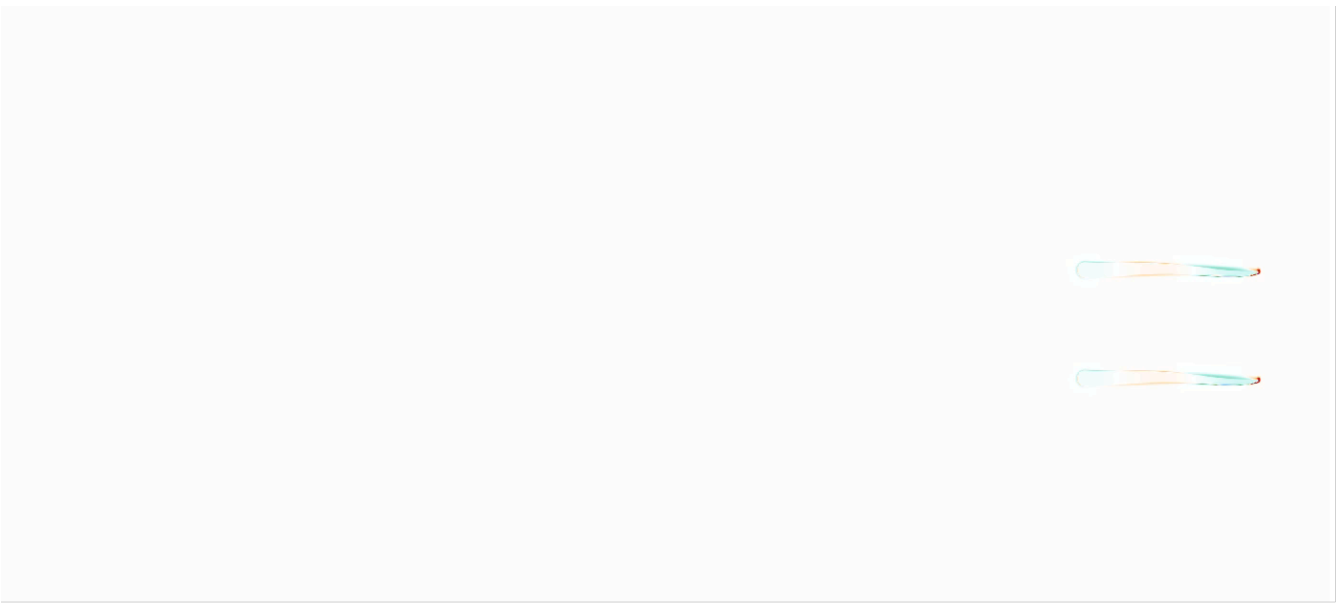
FISH SCHOOLING

?

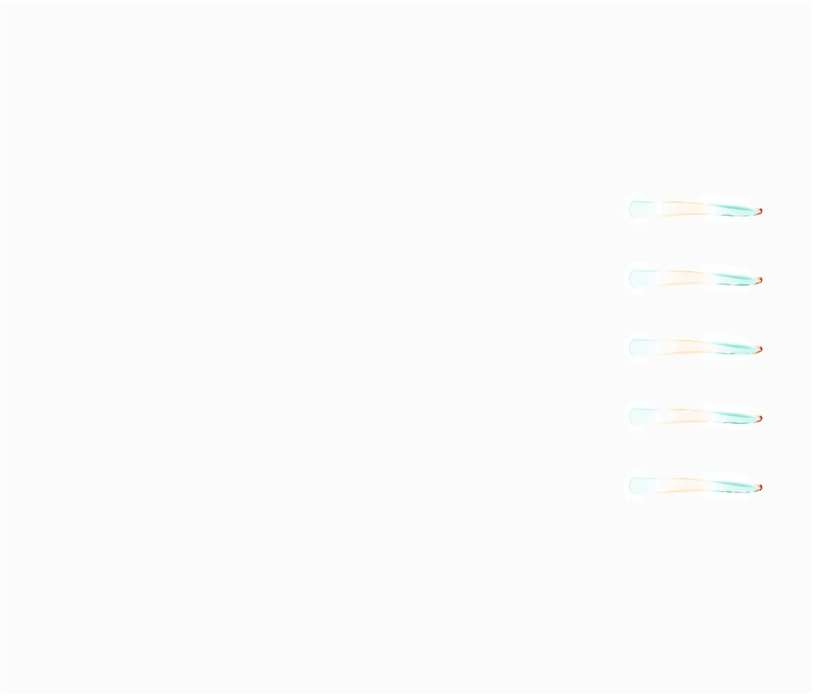
http://www.dailymotion.com/video/xedk1_synchronisedfish

Fixed motion pattern

In order to school, fish modify their motion patterns to cope with changes in the surrounding flow in phase fish

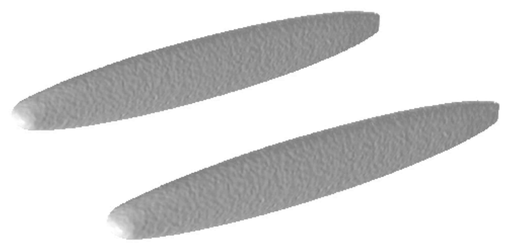


aligned school

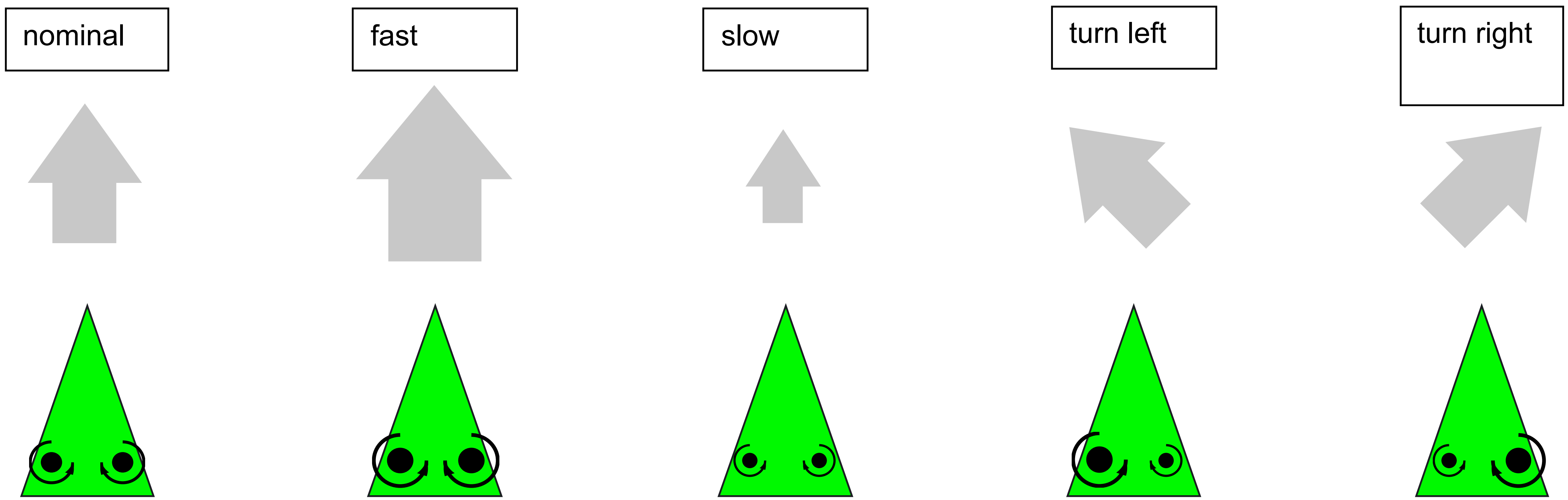


out of phase fish (**π**)(2D)

out of phase fish (**π**)(3D)



Swimmer actions



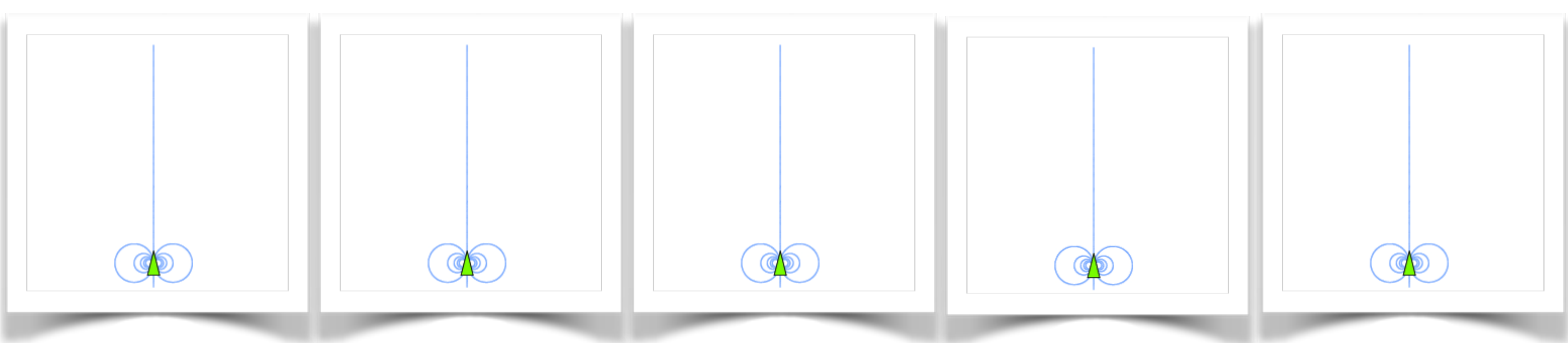
nominal:
$$\Gamma_l = \Gamma_0 \quad \Gamma_r = \Gamma_0 \quad \Gamma_{\text{total}} = 0$$

fast:
$$\Gamma_l = \Gamma_0 + \Gamma_A \quad \Gamma_r = \Gamma_0 + \Gamma_A \quad \Gamma_{\text{total}} = 0$$

slow:
$$\Gamma_l = \Gamma_0 - \Gamma_A \quad \Gamma_r = \Gamma_0 - \Gamma_A \quad \Gamma_{\text{total}} = 0$$

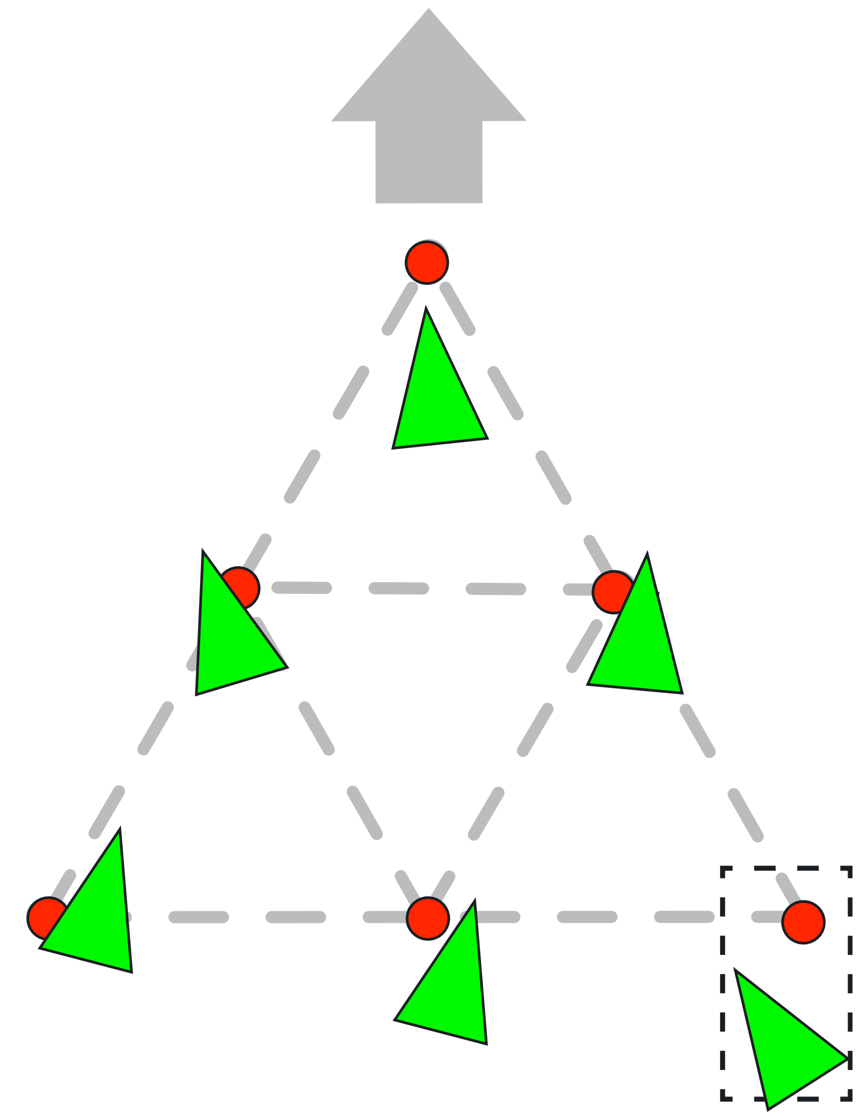
turn left:
$$\Gamma_l = \Gamma_0 + \Gamma_T \quad \Gamma_r = \Gamma_0 - \Gamma_T \quad \Gamma_{\text{total}} > 0$$

turn right:
$$\Gamma_l = \Gamma_0 - \Gamma_T \quad \Gamma_r = \Gamma_0 + \Gamma_T \quad \Gamma_{\text{total}} < 0$$

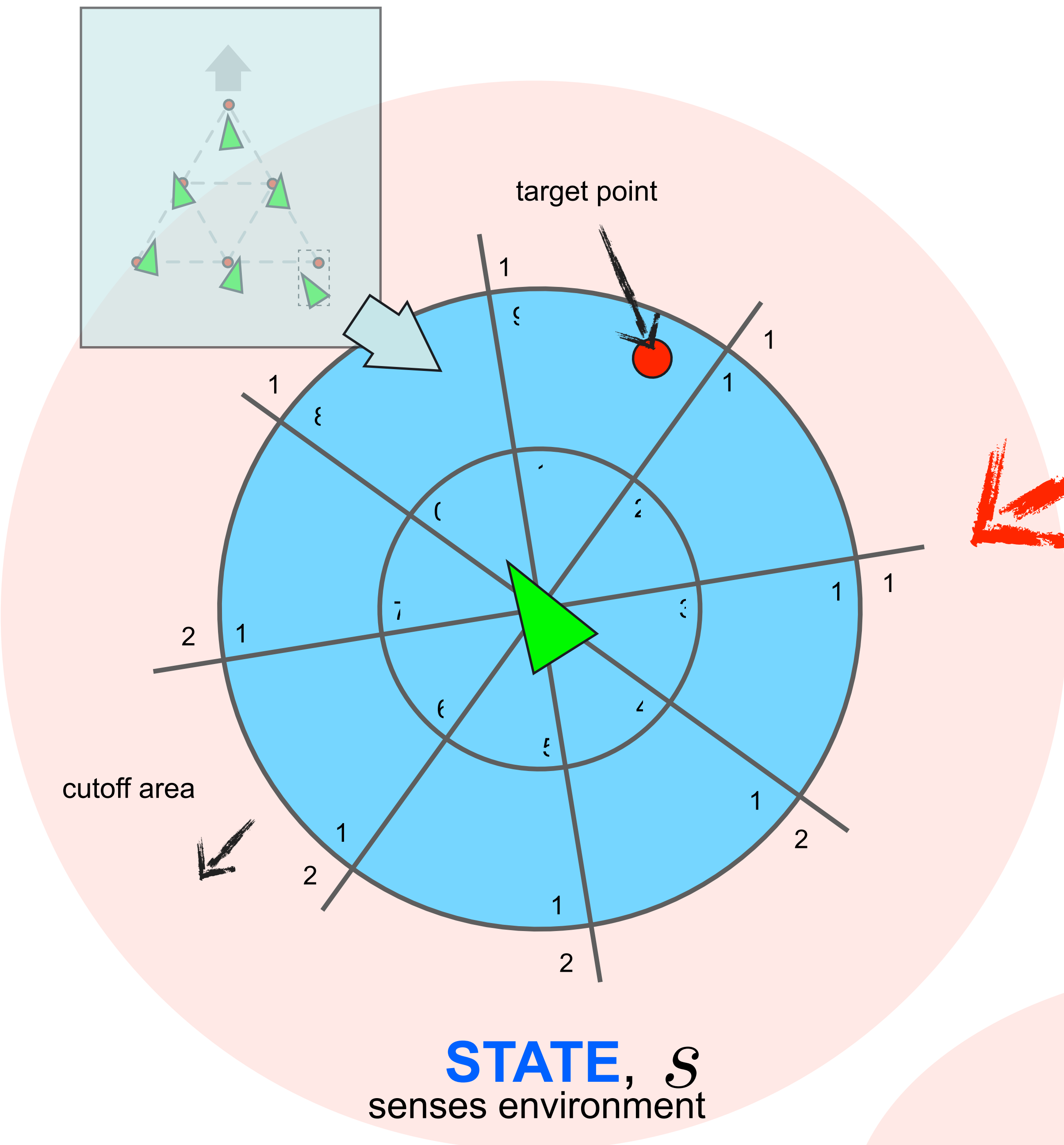


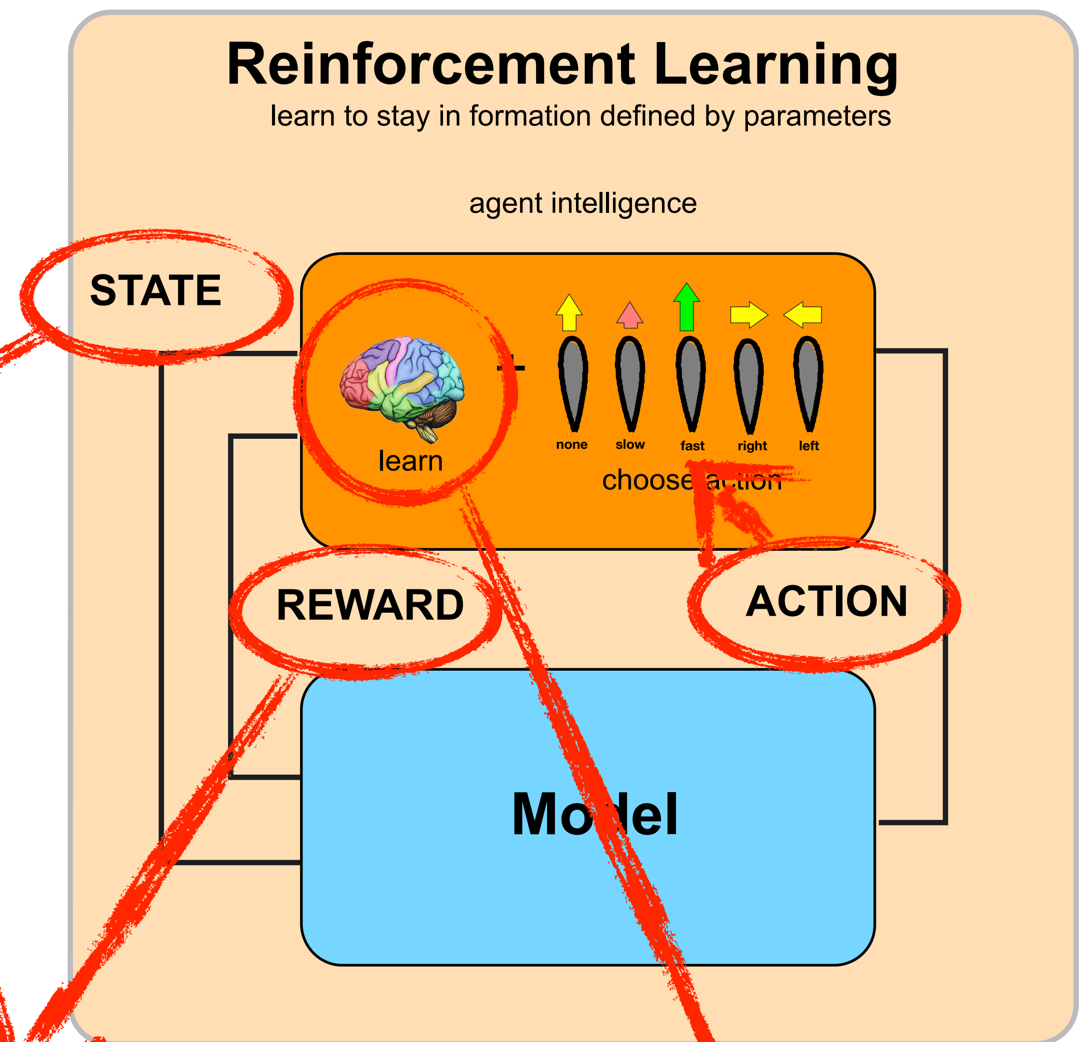
LEARNING

- Follow a point in the lattice
  (we specify it and want to evaluate its effectiveness)



Elements of Reinforcement Learning





REWARD, r
encodes goal

good to be close to target ↓ good to be lazy ↓

$$r = w_\mathrm{d} \cdot (1 - d) + w_\mathrm{a} \cdot \eta(a)$$

where $$\eta(a) = \begin{cases} 1, & \text{if slowing down} \\ 0, & \text{else} \end{cases}$$

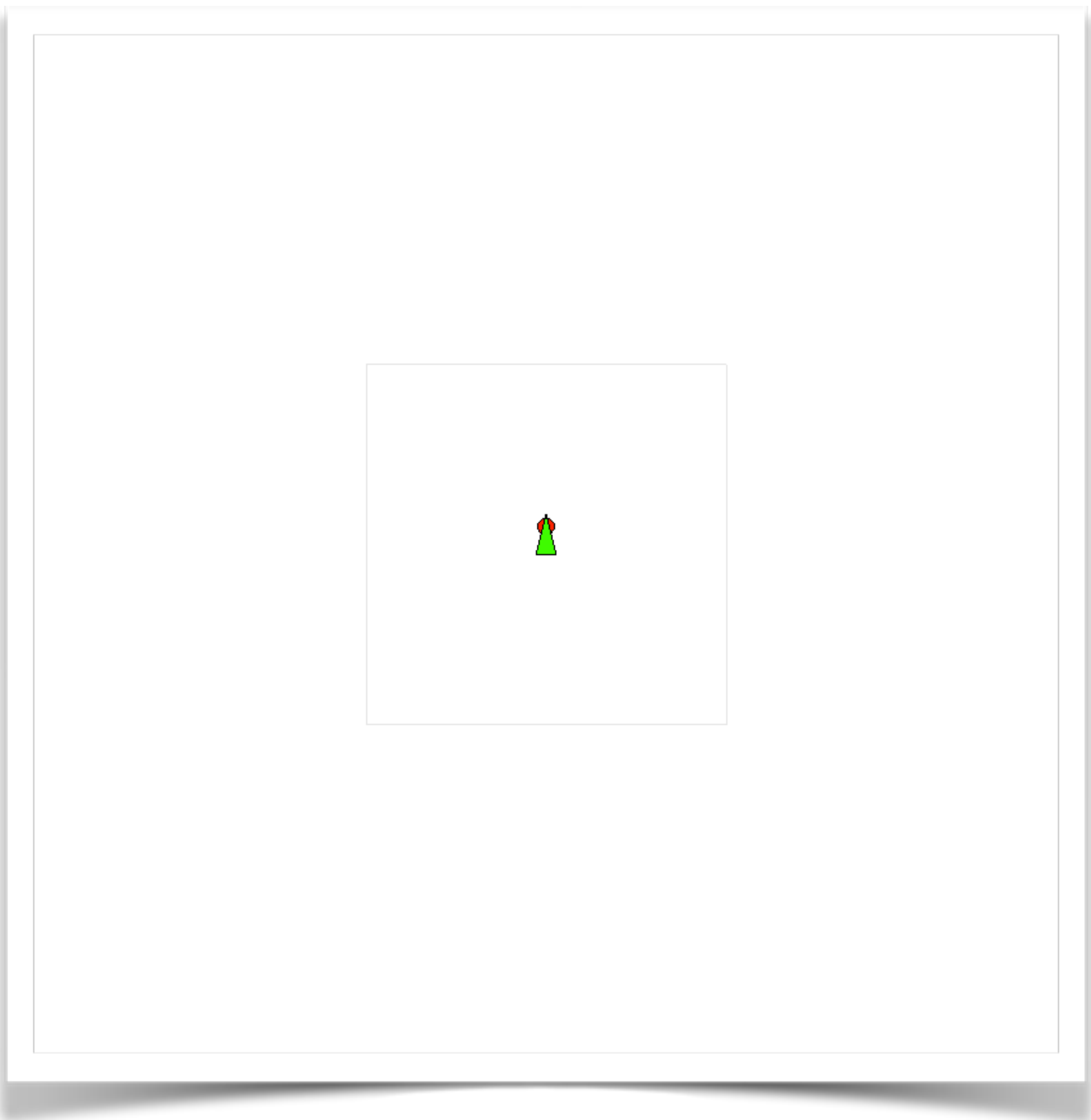
LEARN
by updating
VALUE, $Q(s, a)$
expected long term reward

$$Q(s,a) \leftarrow Q(s,a) + \Delta Q(s,a;r,s')$$

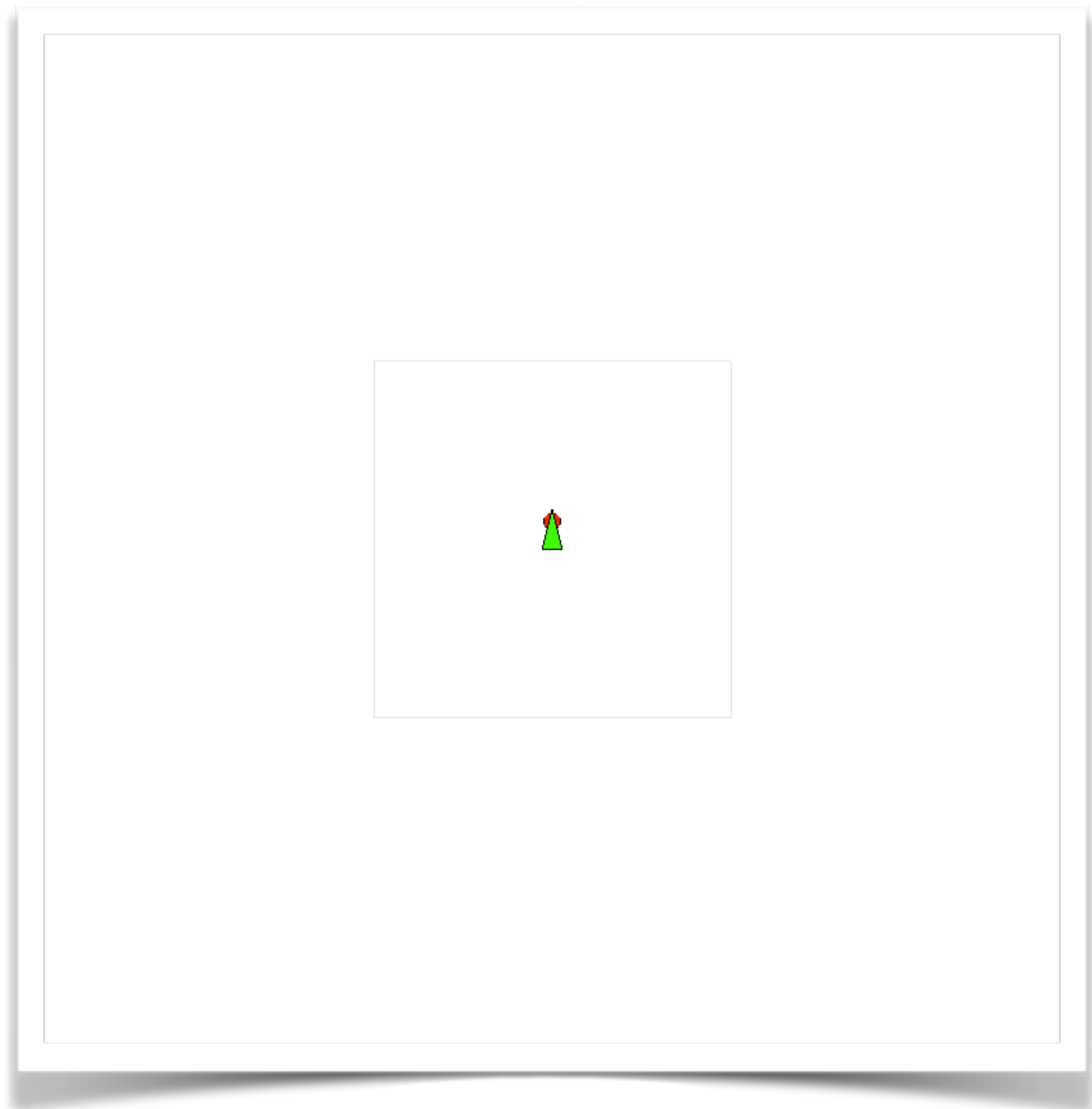
$$\Delta Q(s,a;r,s') = \alpha\left(r + \gamma \max_{a'} Q(s',a') - Q(s,a)\right)$$

Reinforcement Learning

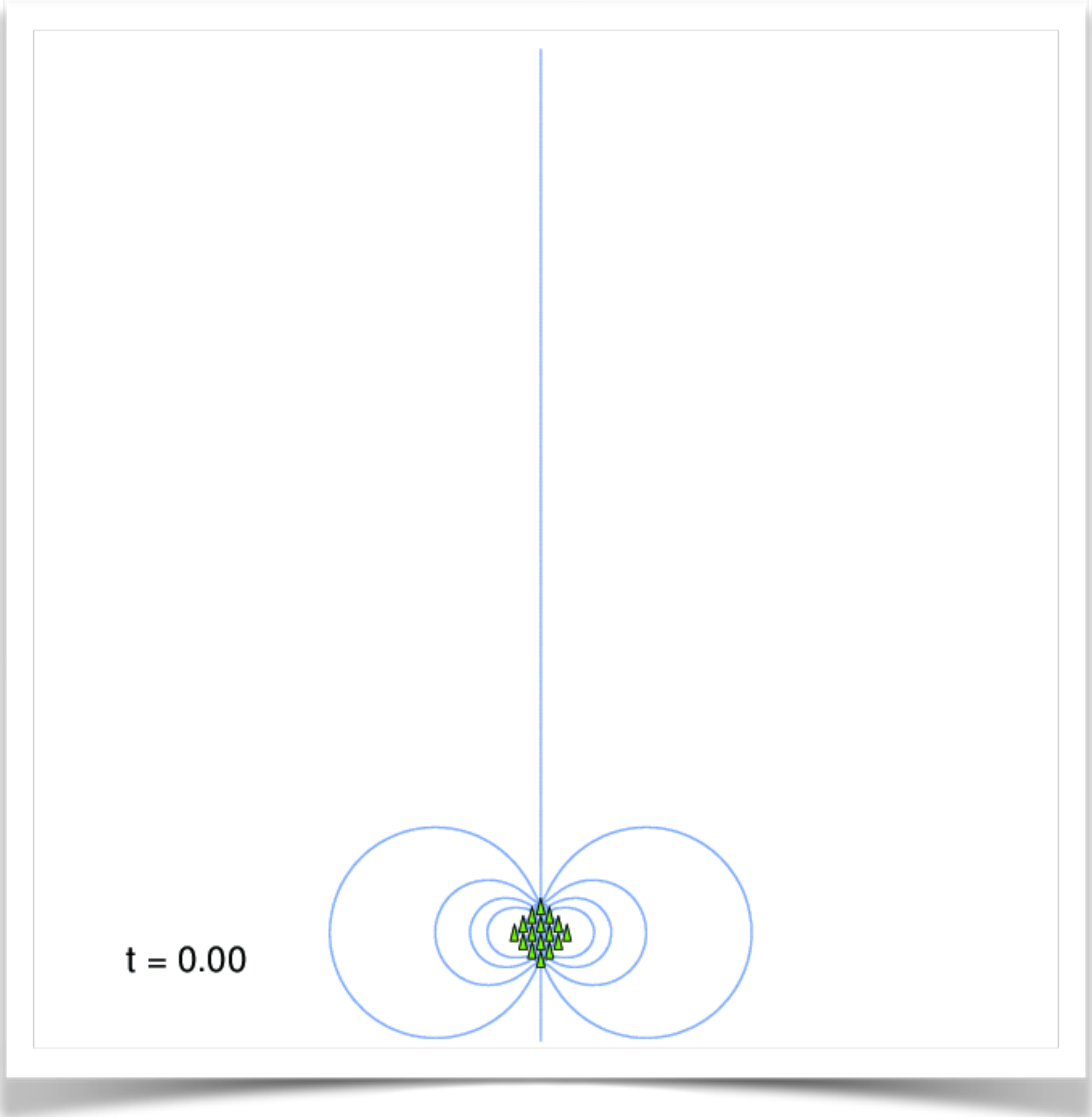
intermediate learning state



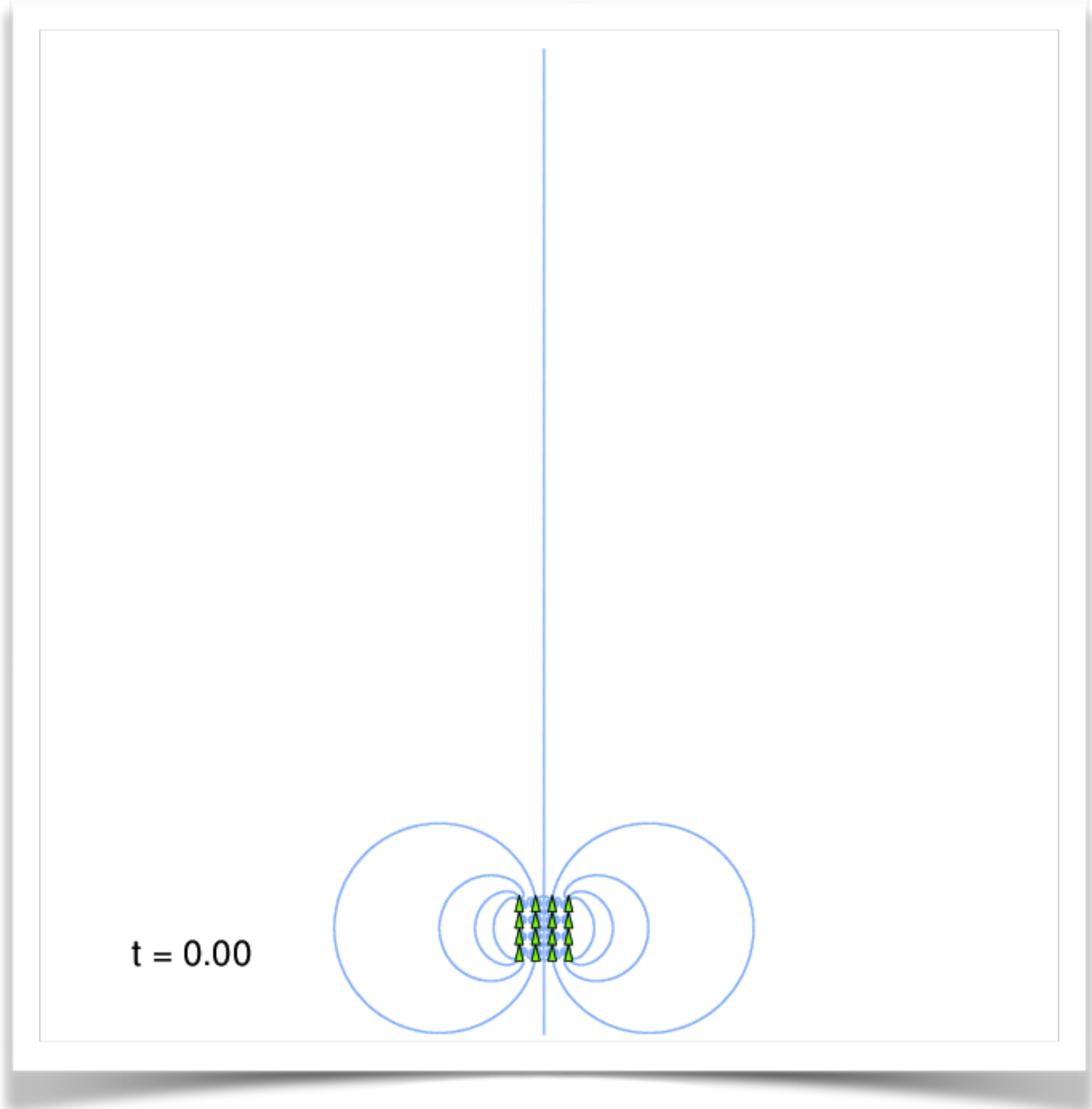
advanced learning state



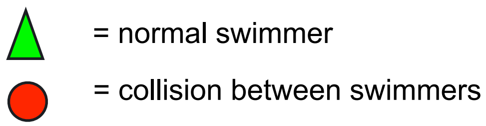
Fixed motion swimmers



initially diamond-like formation

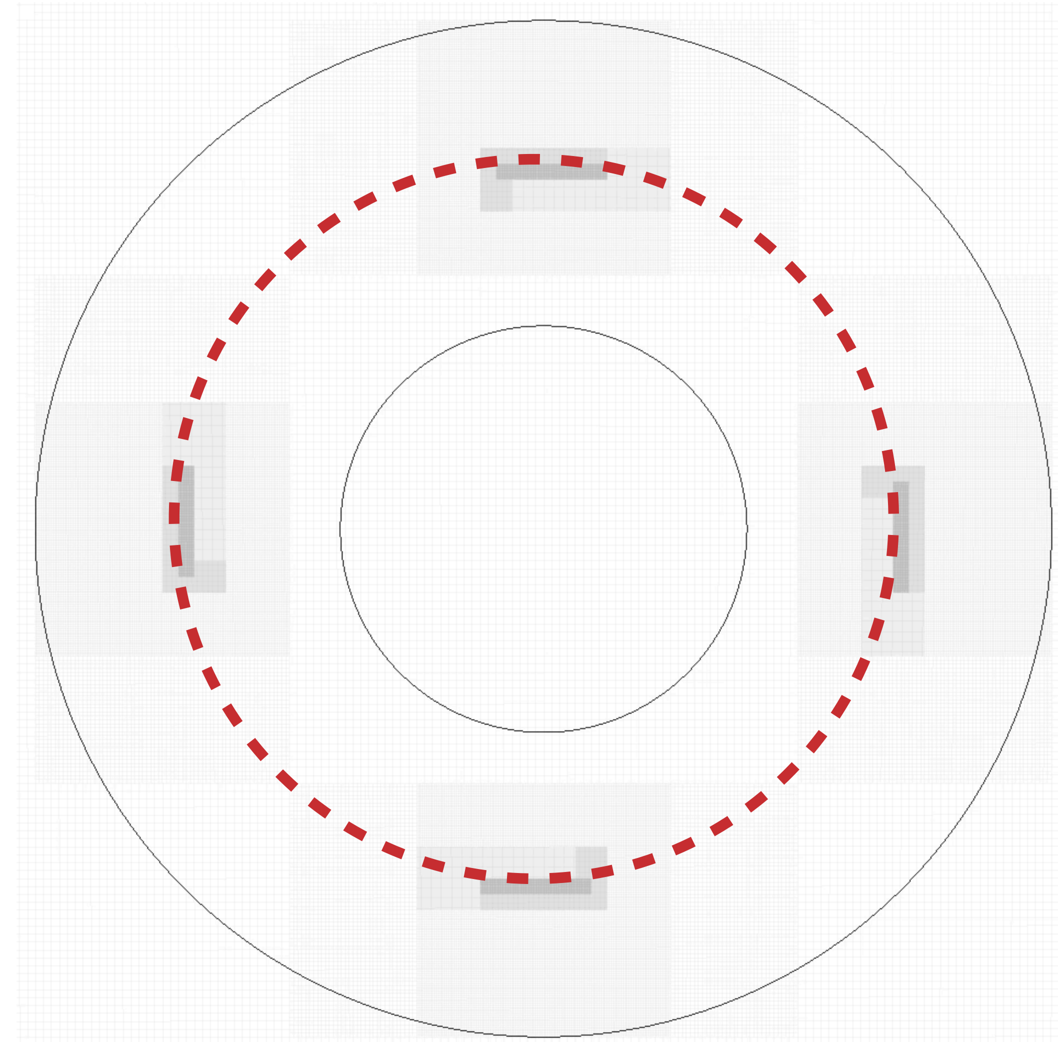


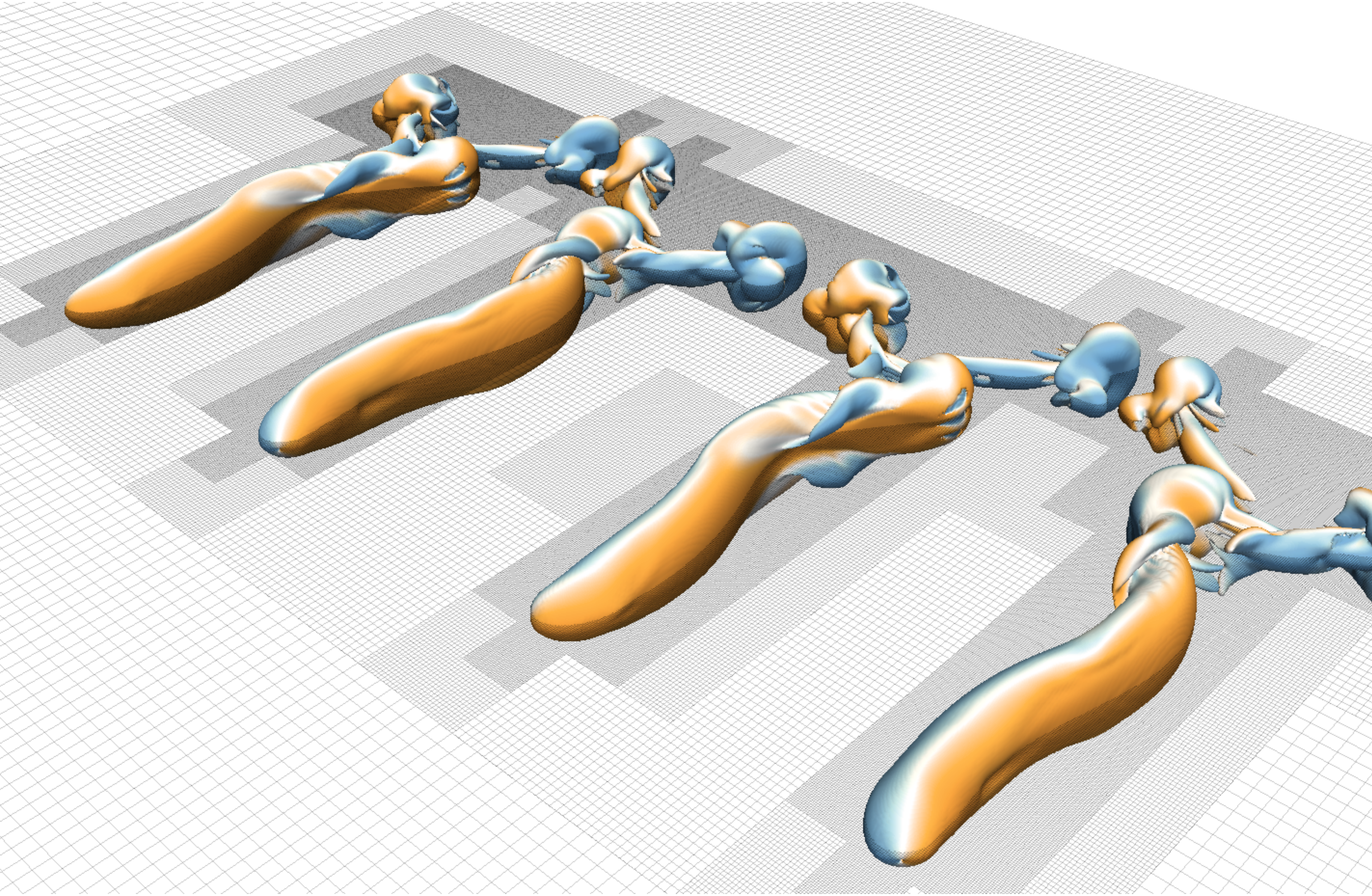
initially square-like formation



Learning to swim together

• 5 motions: straight, left, right, **speed up, slow down**





Thank you