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Tackling real-world problems with modern software

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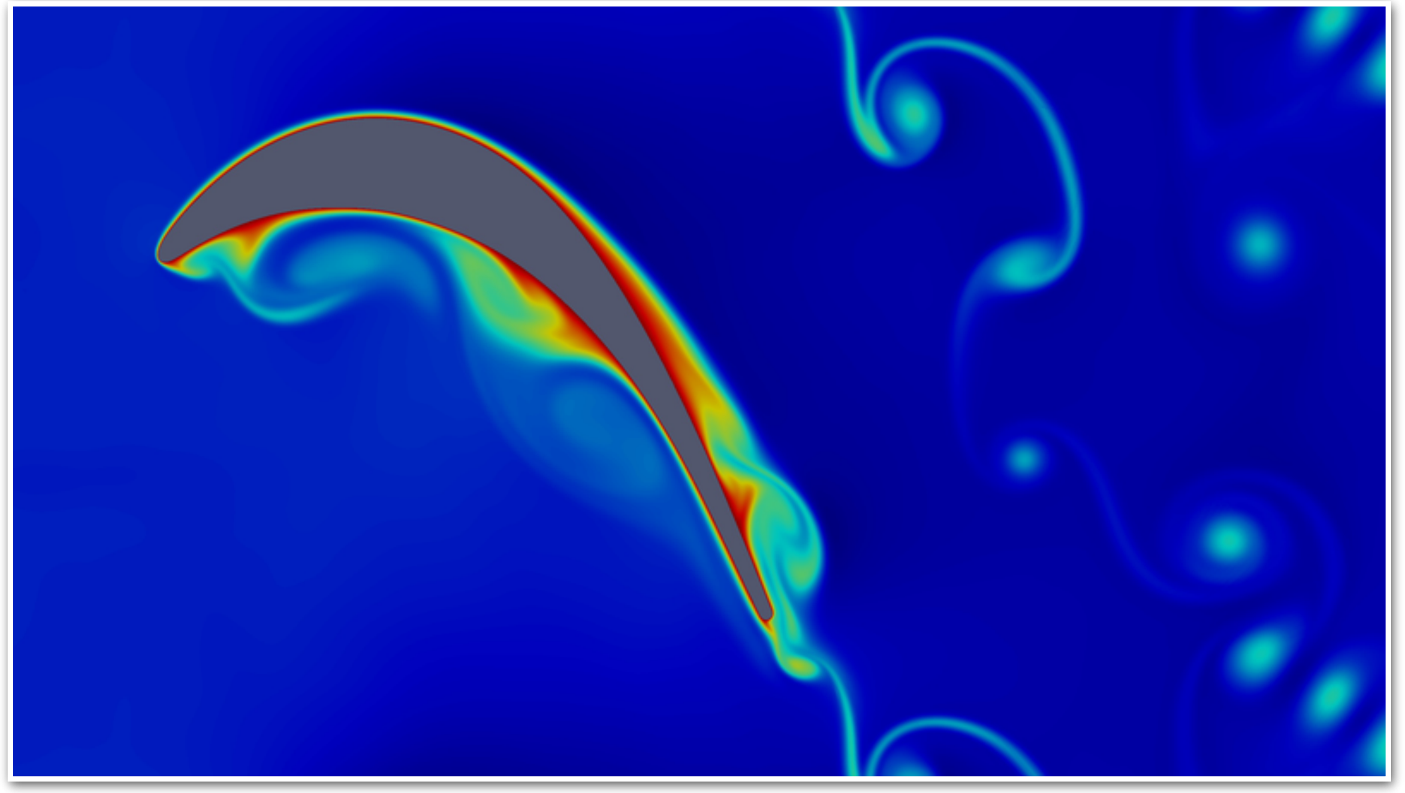
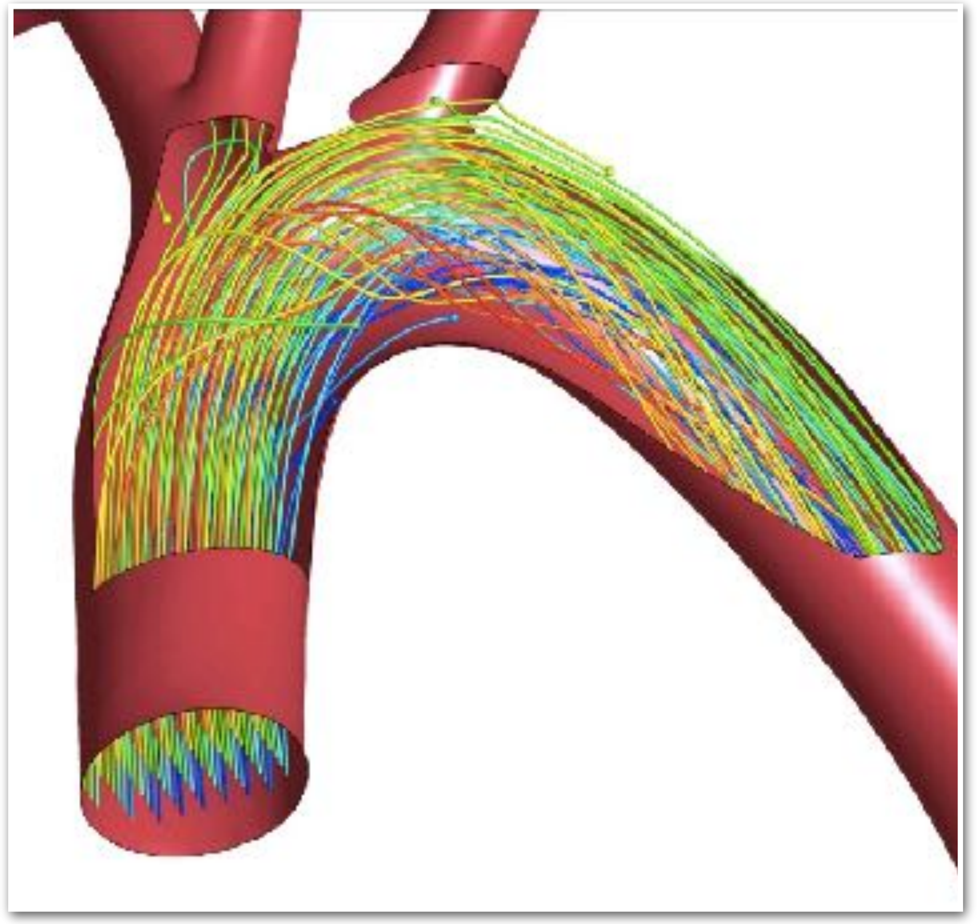
Overview

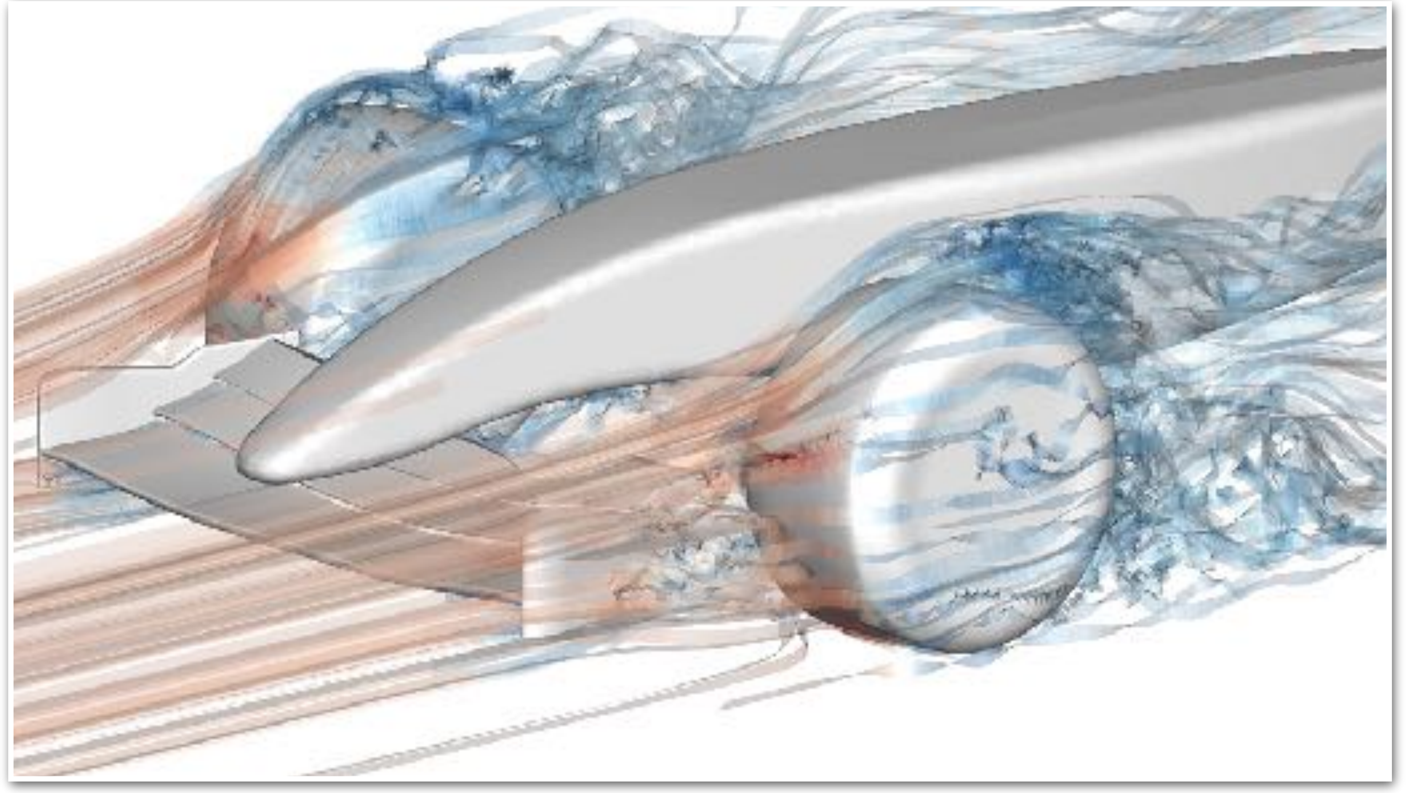
- Computational modelling plays a key role in many scientific fields.
- The increasing power of computing hardware means:
  - ➡ more detailed simulations, finer resolution of physics;
  - ➡ look at wider ranges of parameters.
- Today I'll talk about two fairly disconnected fields: fluid dynamics & cardiac electrophysiology.
- How do we design software that's flexible enough to tackle multiple areas & can exploit power on offer?



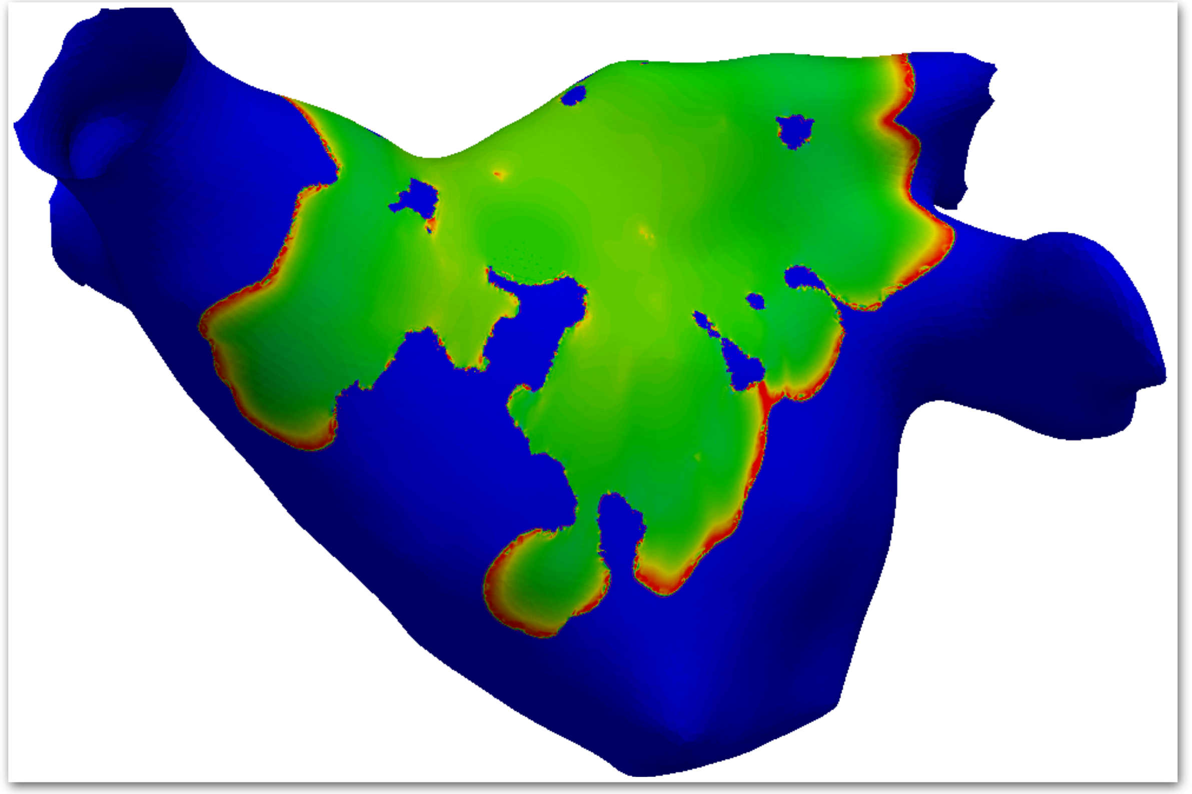
aviation and aerospace



bioflows & bioengineering



motorsport



cardiac electrophysiology

Lombard, Moxey et al., *AIAA J* (2016)

Increasing desire for **high-fidelity** simulation in high-end engineering applications.

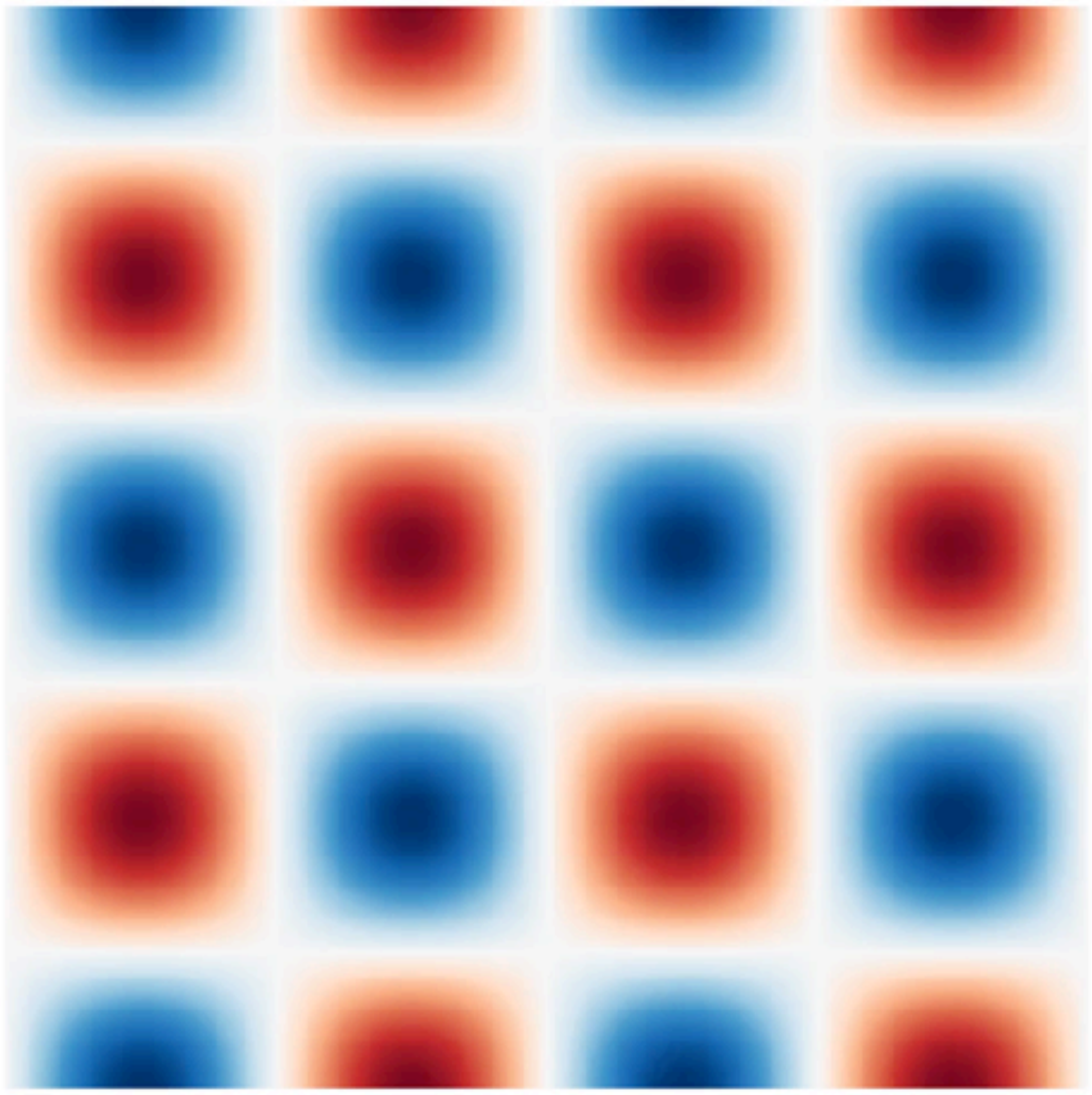
Want to accurately model difficult features:

- strongly separated flows
- feature tracking and prediction
- vortex interaction

Computational power is nearly there: now we need the software to drive this.

How do we model a physical system?

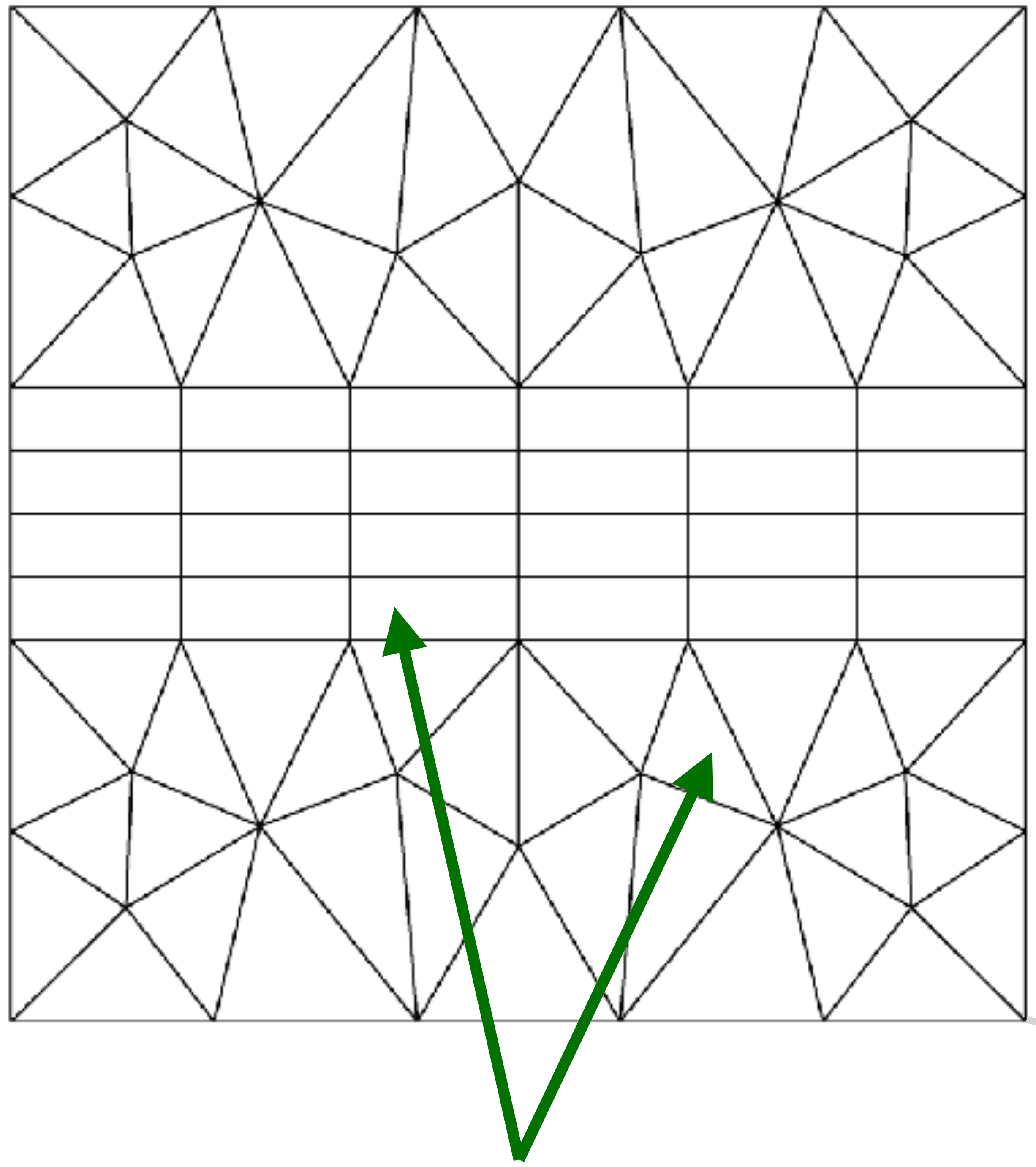
form underlying equations



advection velocity $\mathbf{v}$

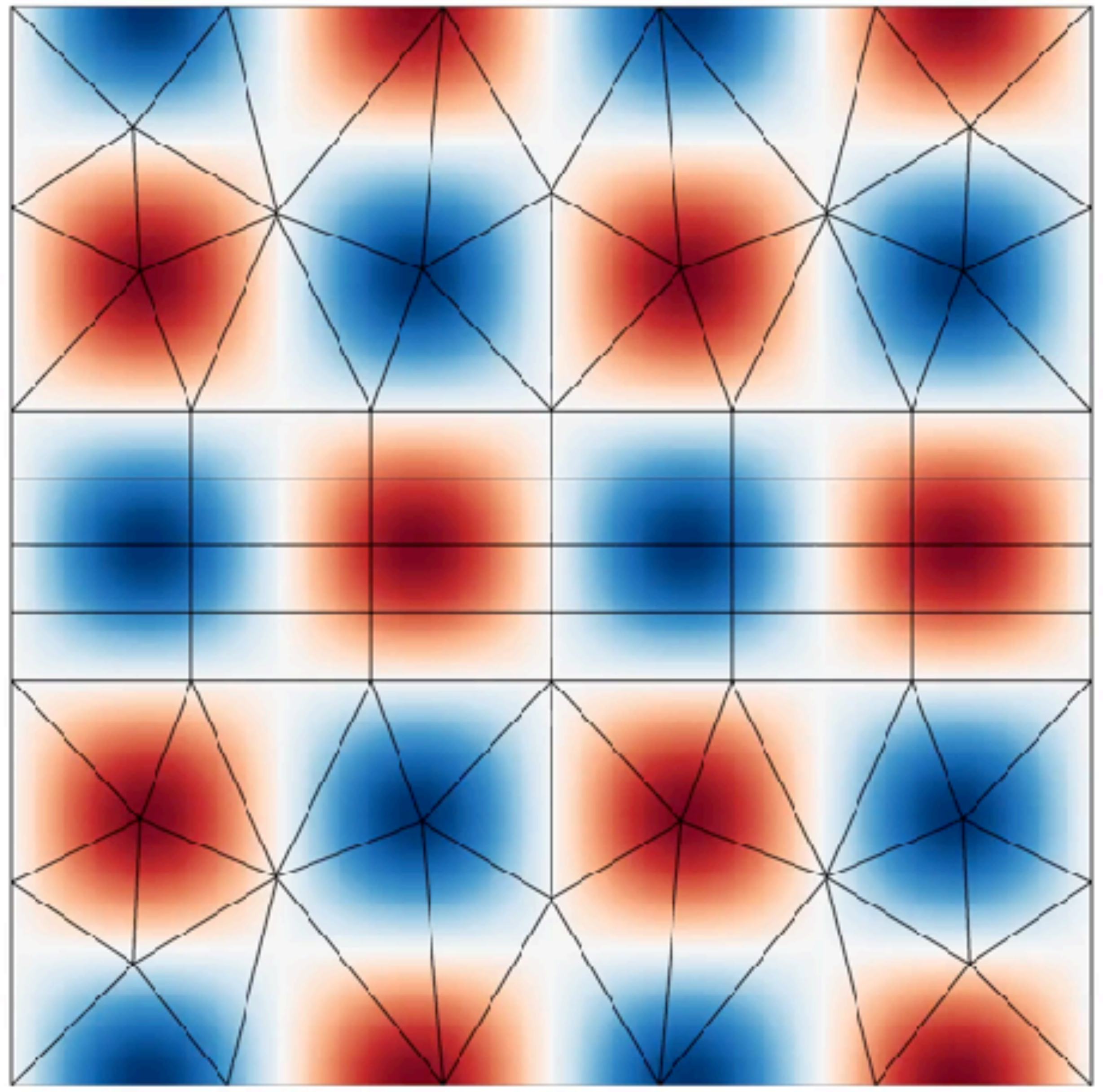
$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = 0$$

discretise (sometimes) complex domain



simpler *elements* on which the equations can be solved

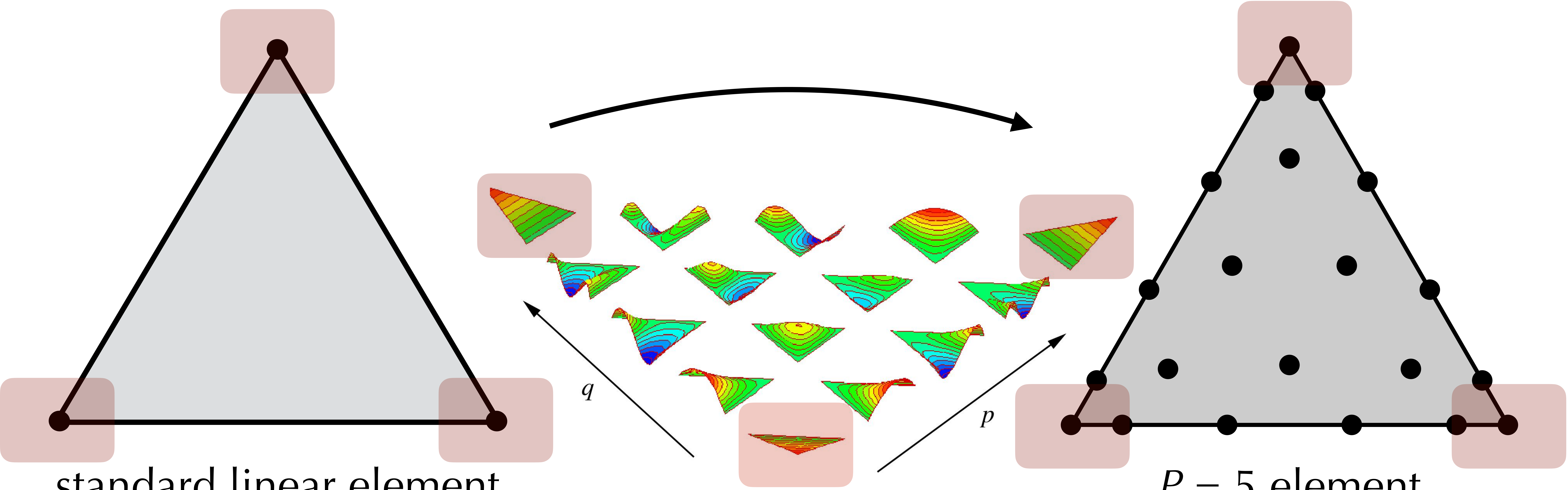
solve resulting system



$$\mathbf{Ax} = \mathbf{b}$$

(+ timestepping)

What is a high-order method?

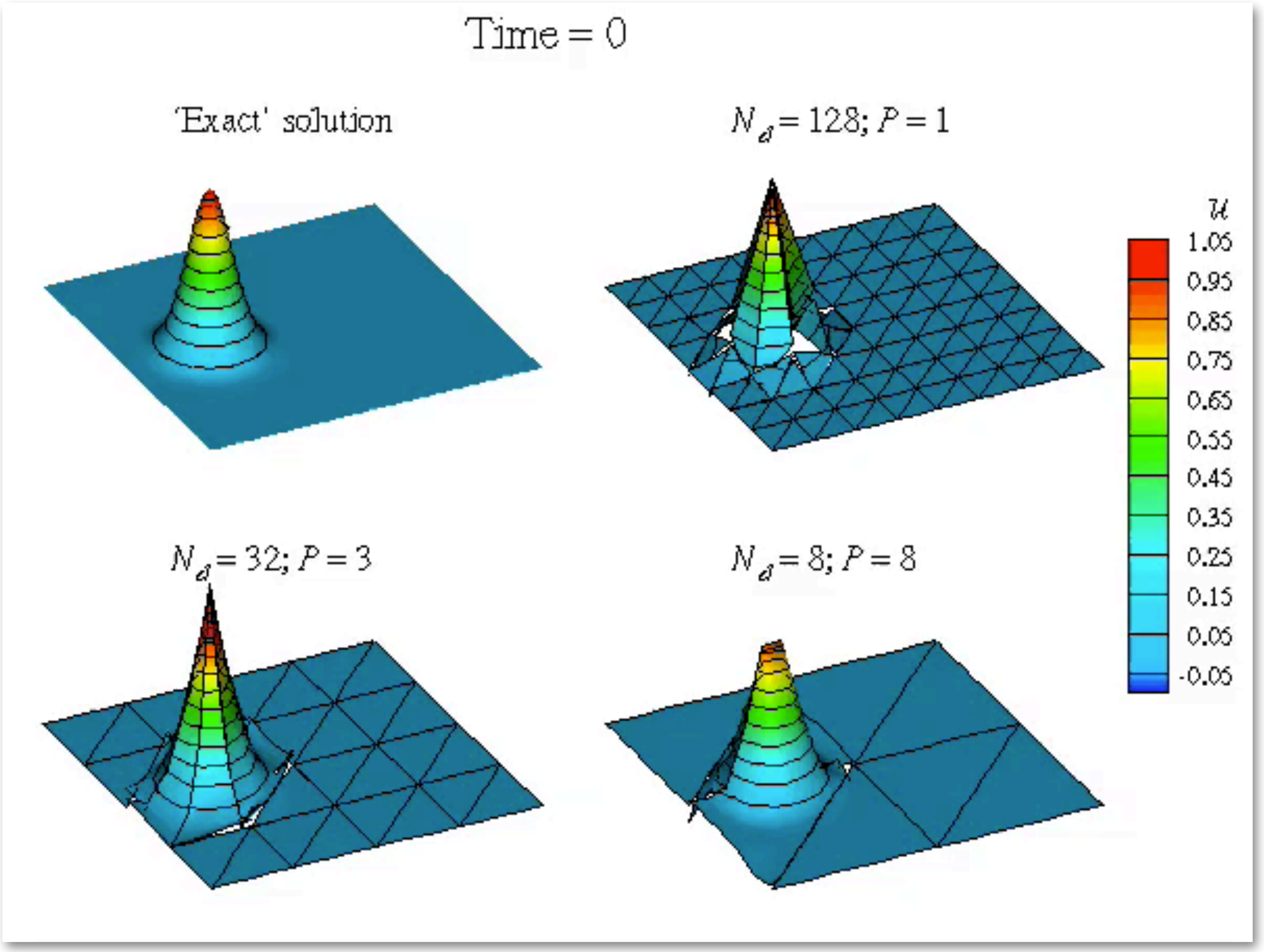


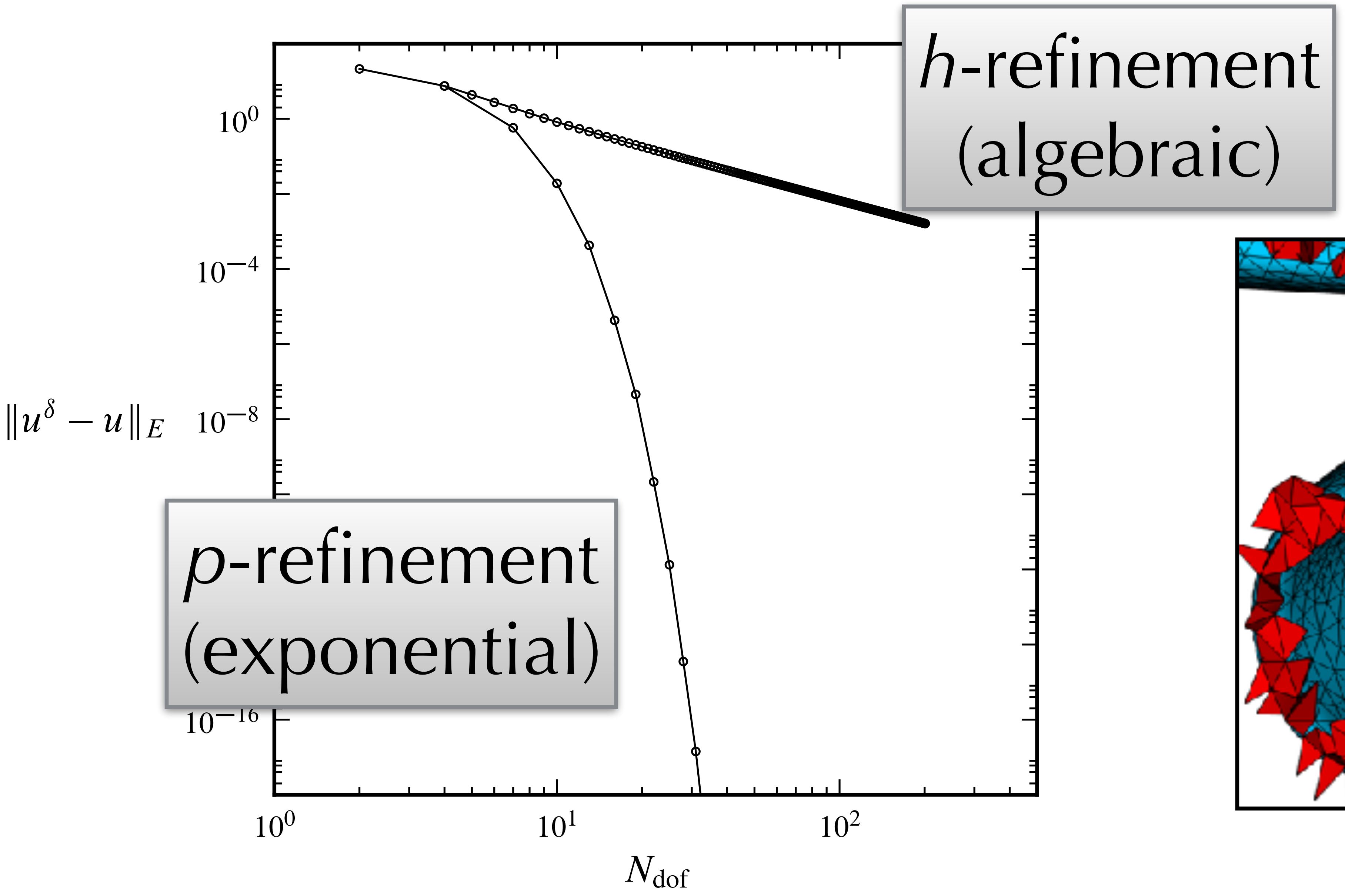
standard linear element
3 degrees of freedom
one per vertex (or cell)

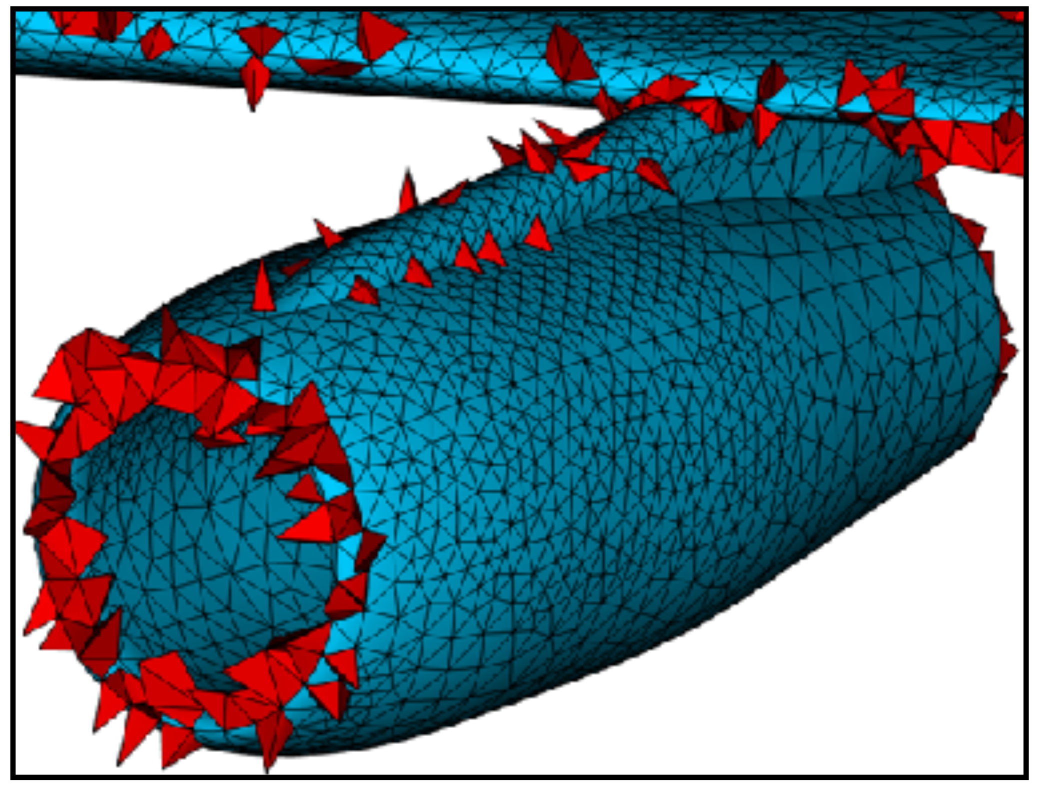
$P = 5$ element
21 degrees of freedom
vertex, edge and interior ‘modes’

Why use a high-order method?

- ✓ error decays *exponentially* (smooth solutions);
- ✓ favorable diffusion & dispersion characteristics;
- ✓ model complex domains
- ✓ computational advantage: reduced memory bandwidth, better use of hardware.







Modelling fluids: high-order splitting scheme

Navier–Stokes:

$$\partial_t \mathbf{u} + \mathbf{N}(\mathbf{u}) = -\nabla p + \nu \nabla^2 \mathbf{u}$$
$$\nabla \cdot \mathbf{u} = 0$$

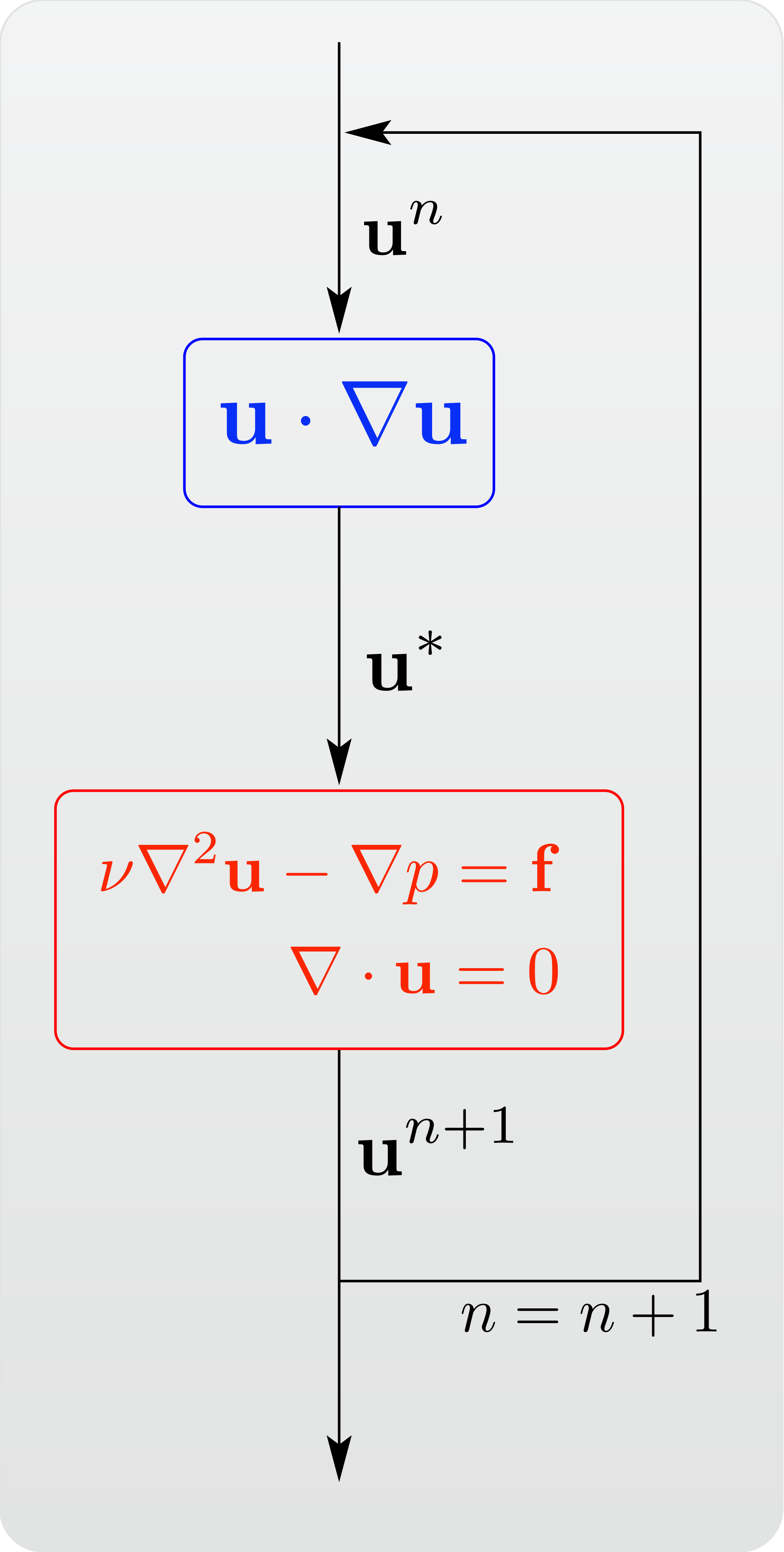
Velocity correction scheme *(aka stiffly stable)*:

Orszag, Israeli, Deville (90), Karnaidakis Israeli, Orszag (1991), Guermond & Shen (2003)

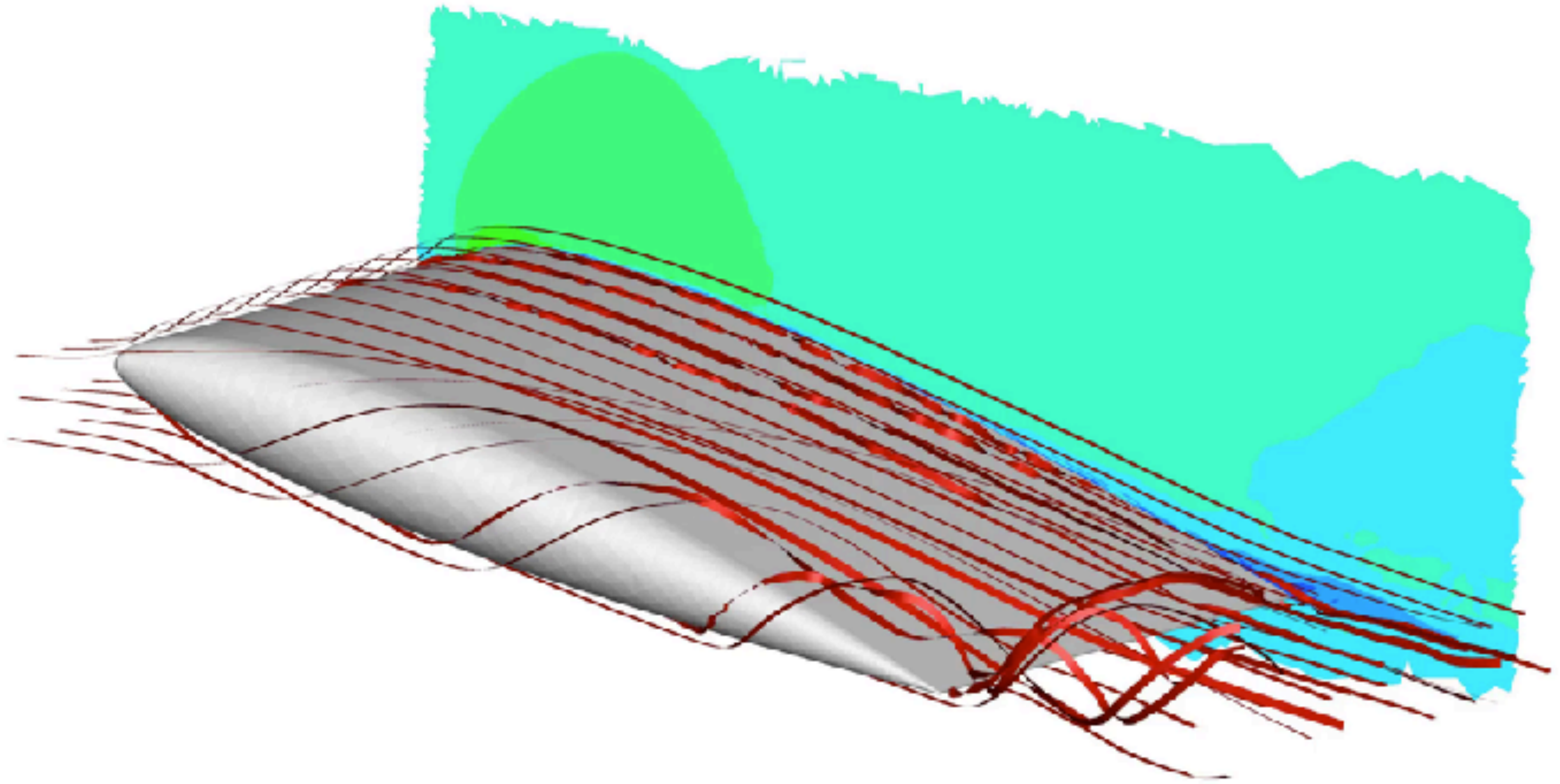
Advection: $$u^* = -\sum_{q=1}^{J} \alpha_q \mathbf{u}^{n-q} - \Delta t \sum_{q=0}^{J-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q})$$

Pressure Poisson: $$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^*$$

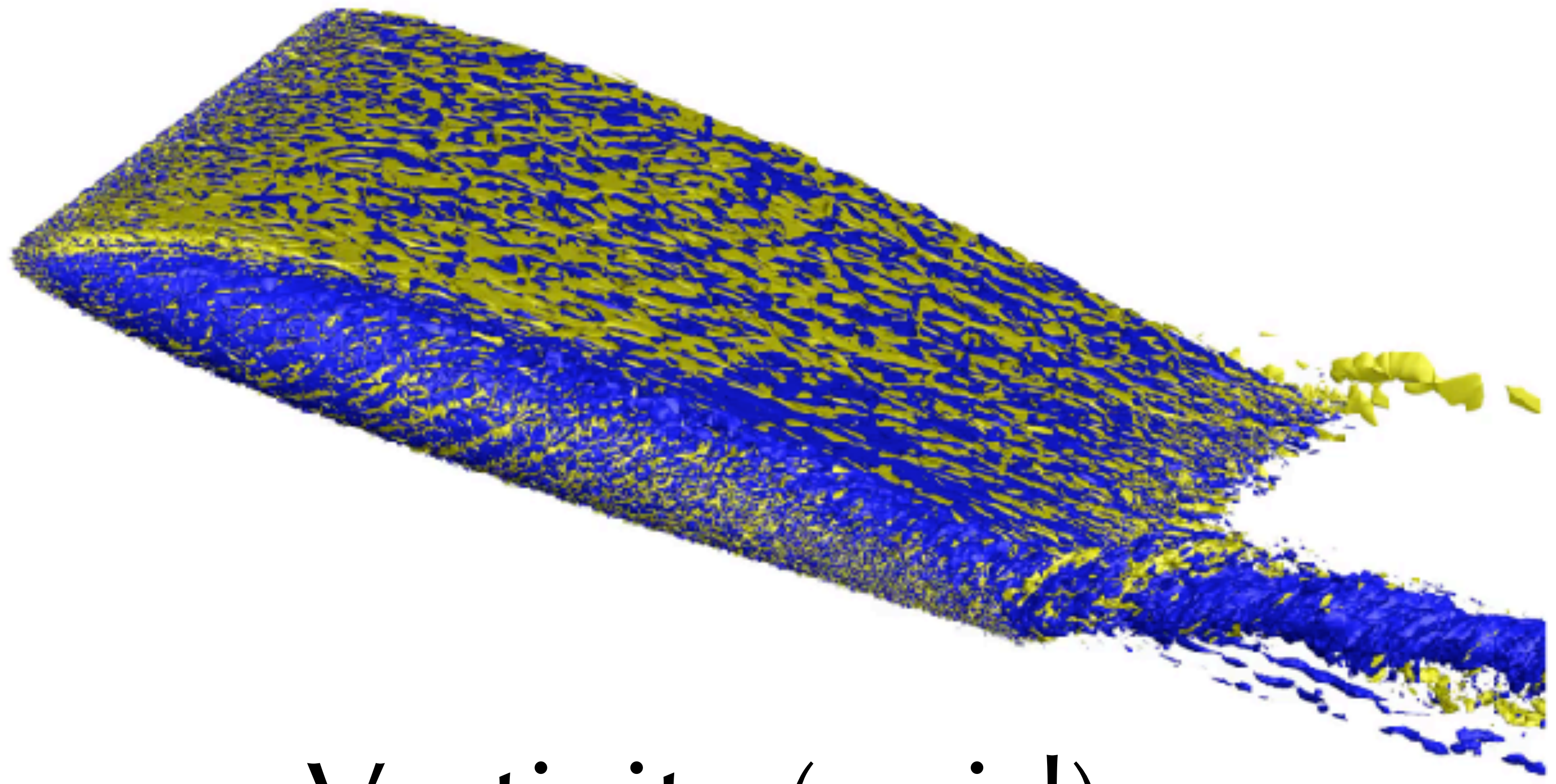
Helmholtz: $$\nabla^2 \mathbf{u}^{n+1} - \frac{\alpha_0}{\nu \Delta t} \mathbf{u}^{n+1} = -\frac{\mathbf{u}^*}{\nu \Delta t} + \frac{1}{\nu} \nabla p^{n+1}$$



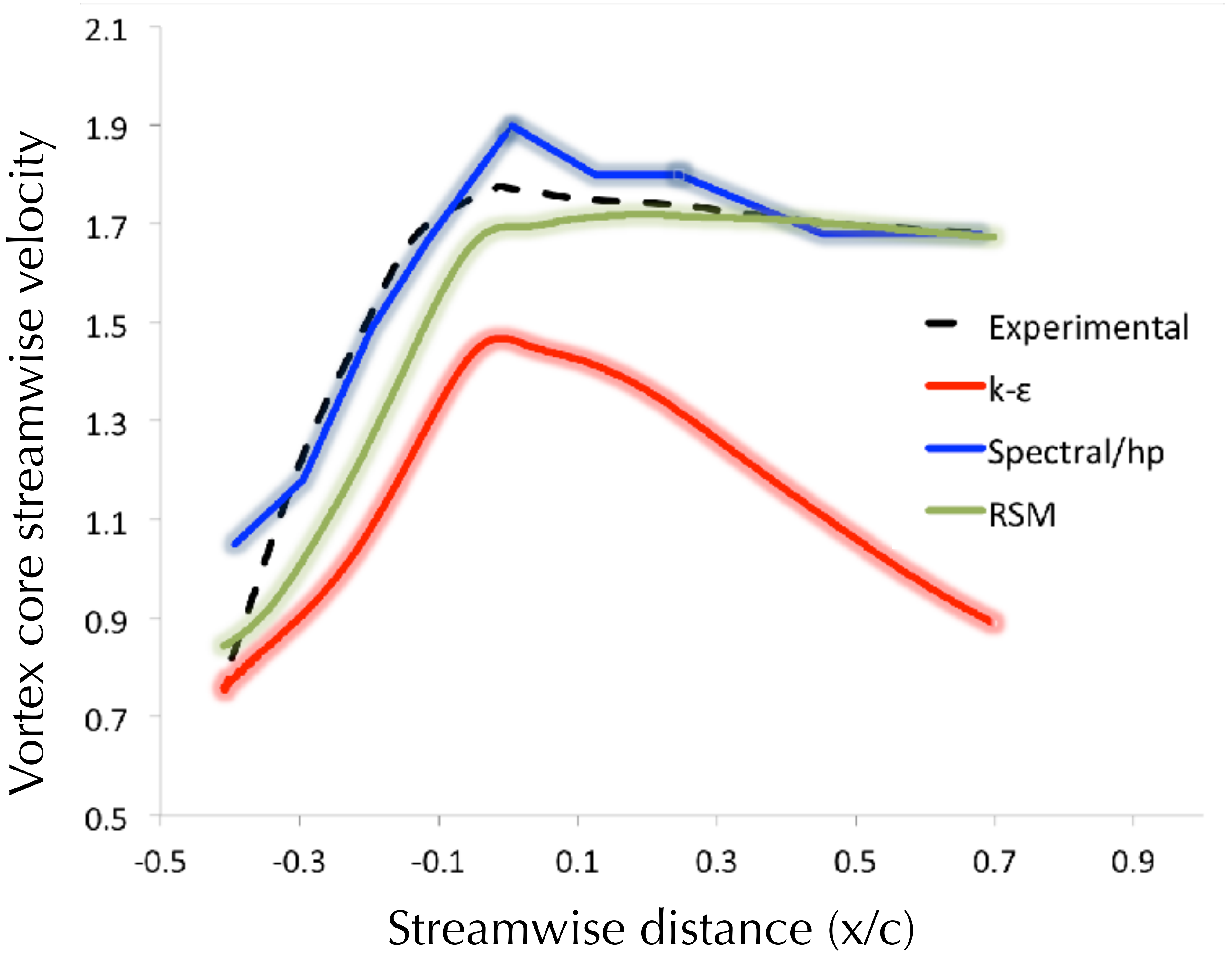
Results on the wingtip simulation



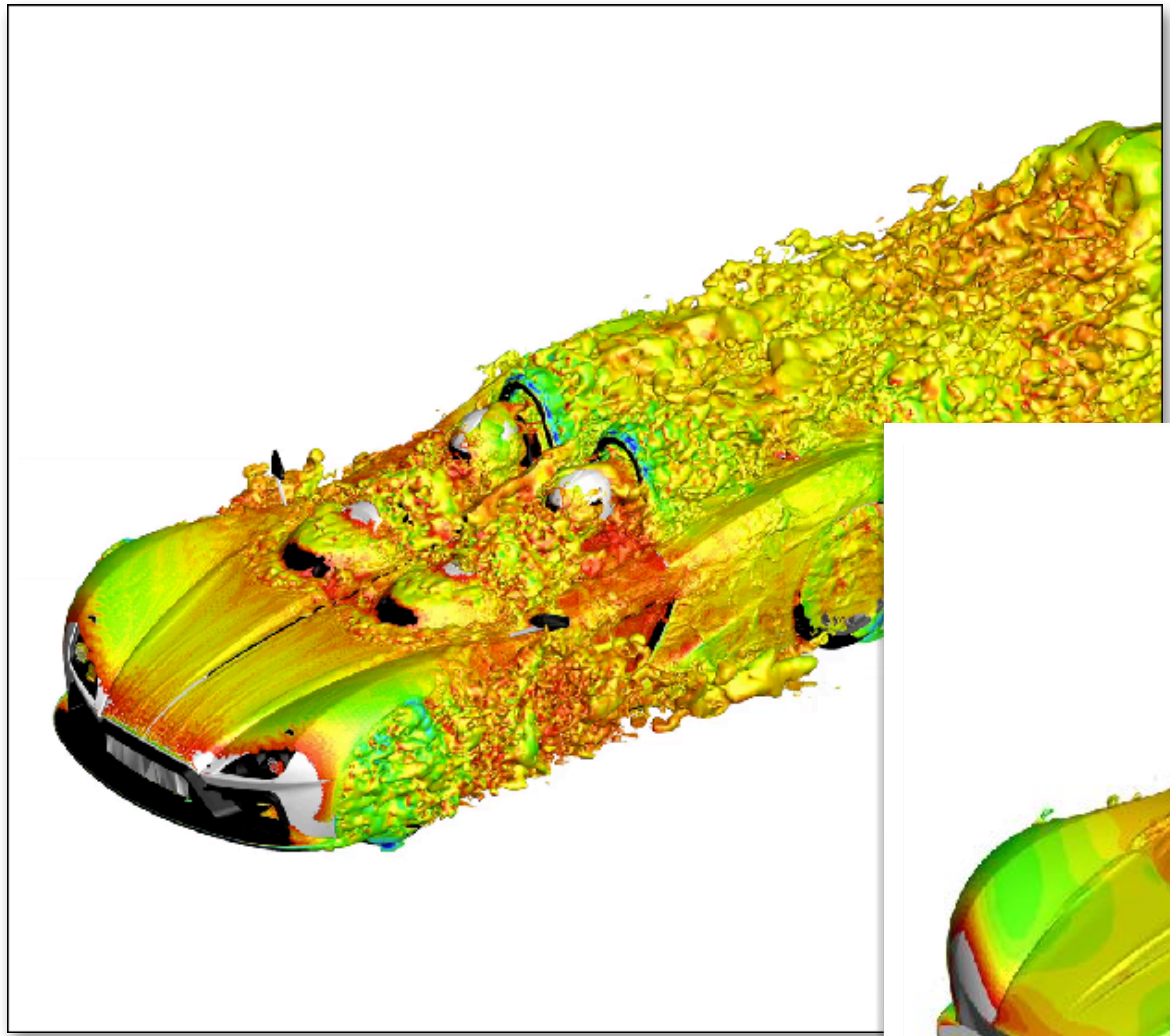
Streamlines



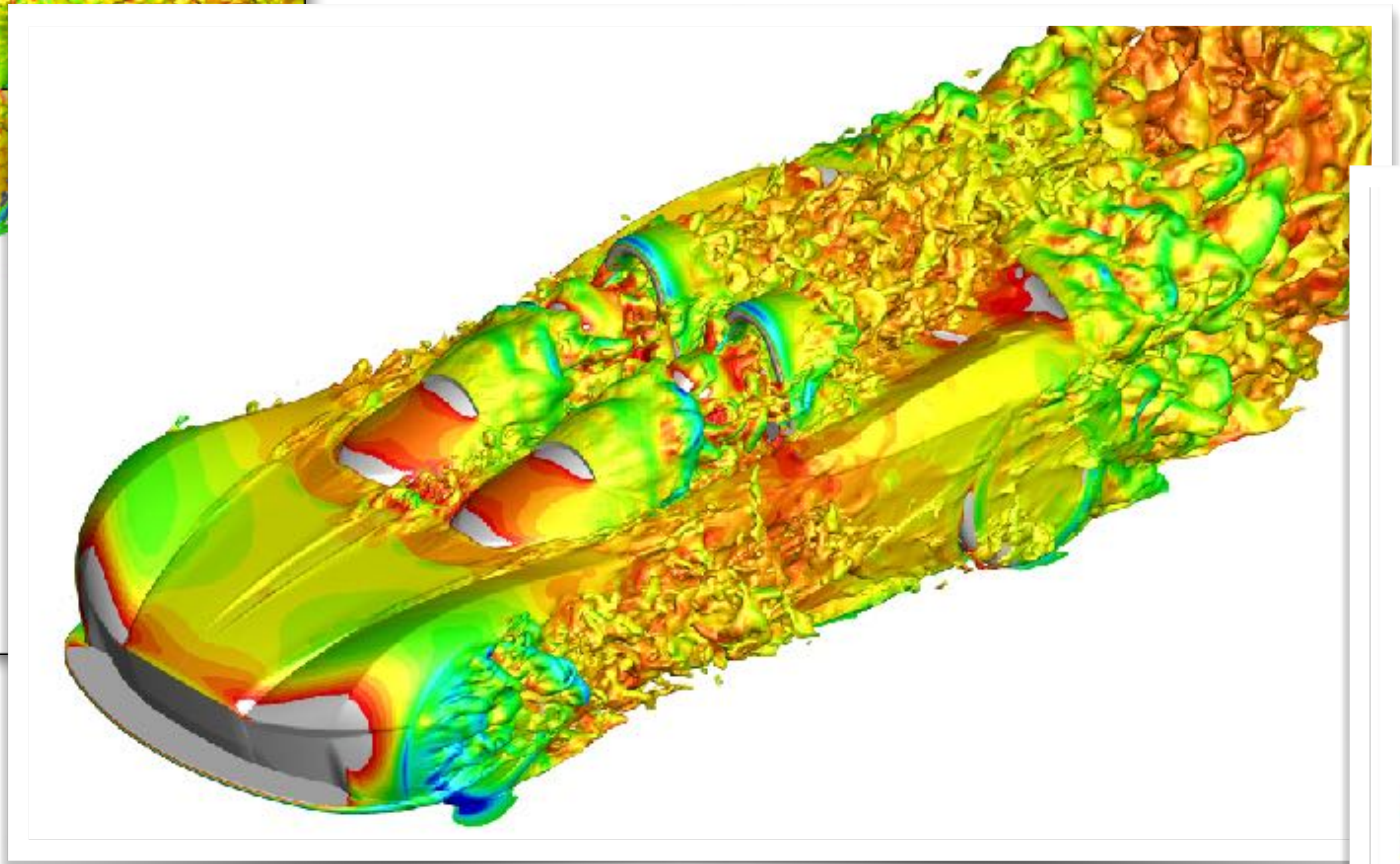
Vorticity (swirl)



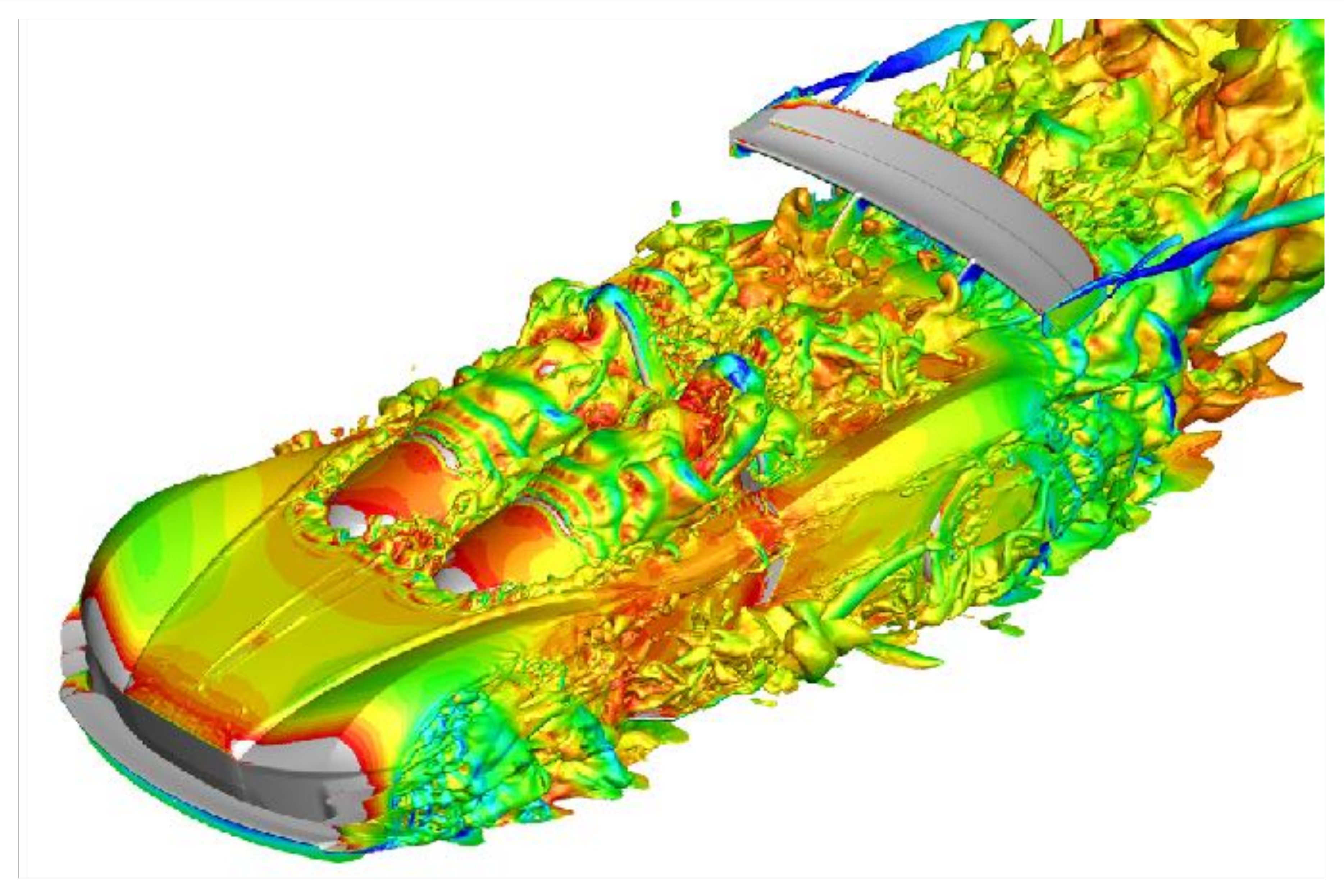
More complex: Elemental road race car



1bn degrees of freedom
Use solely CFD for design



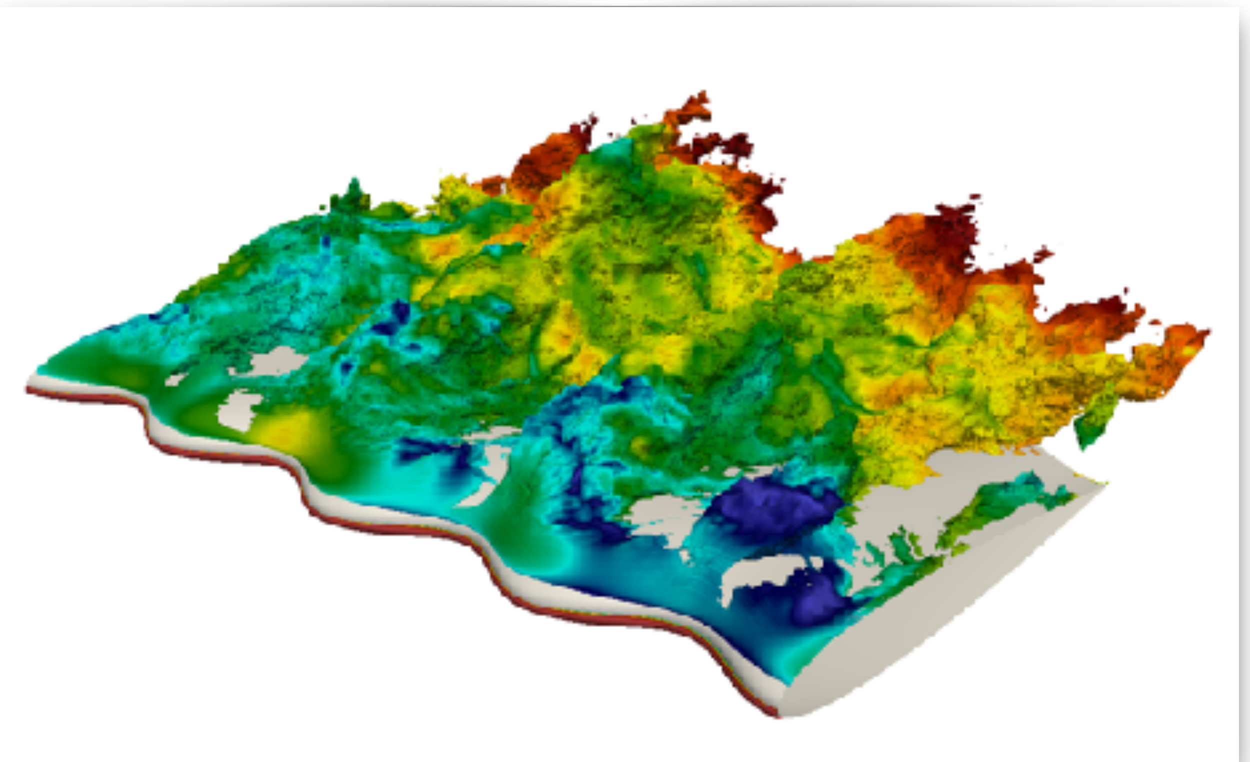
Design 2: +33% Downforce



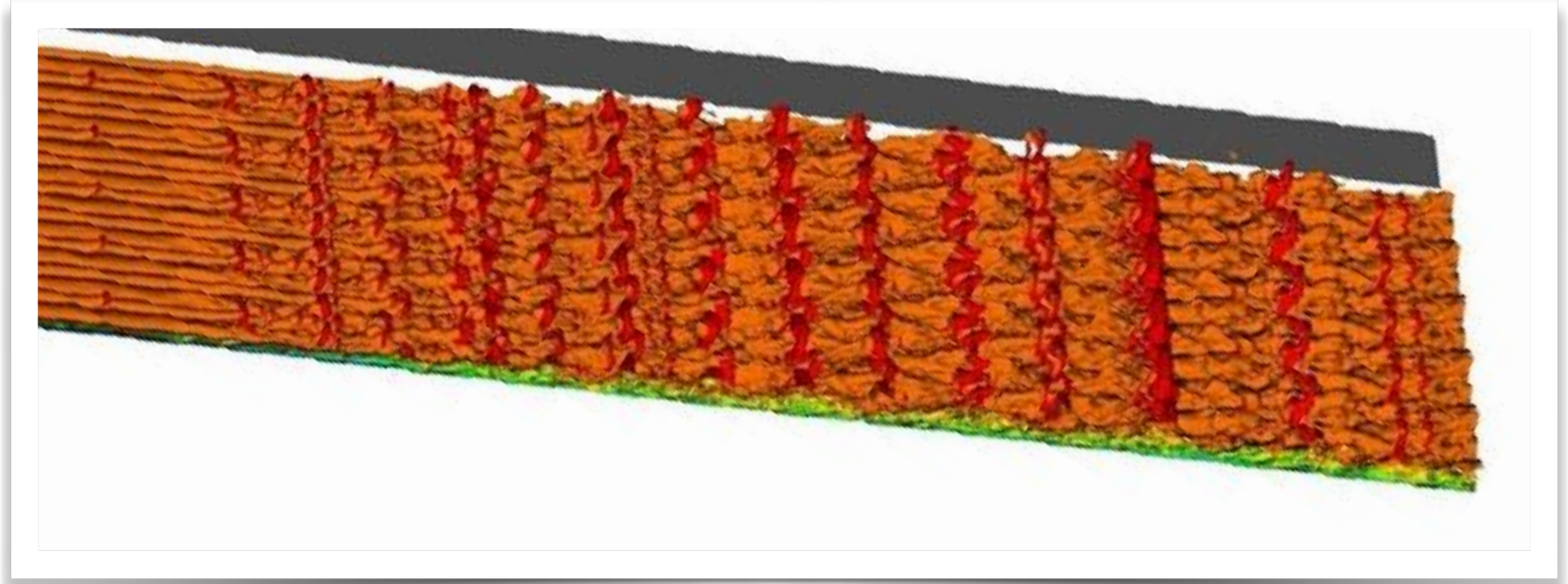
Design 3: +270% Downforce

Mengaldo, Moxey, Turner, Jassim, Taylor, Peiro & Sherwin: arXiv:2009.10178

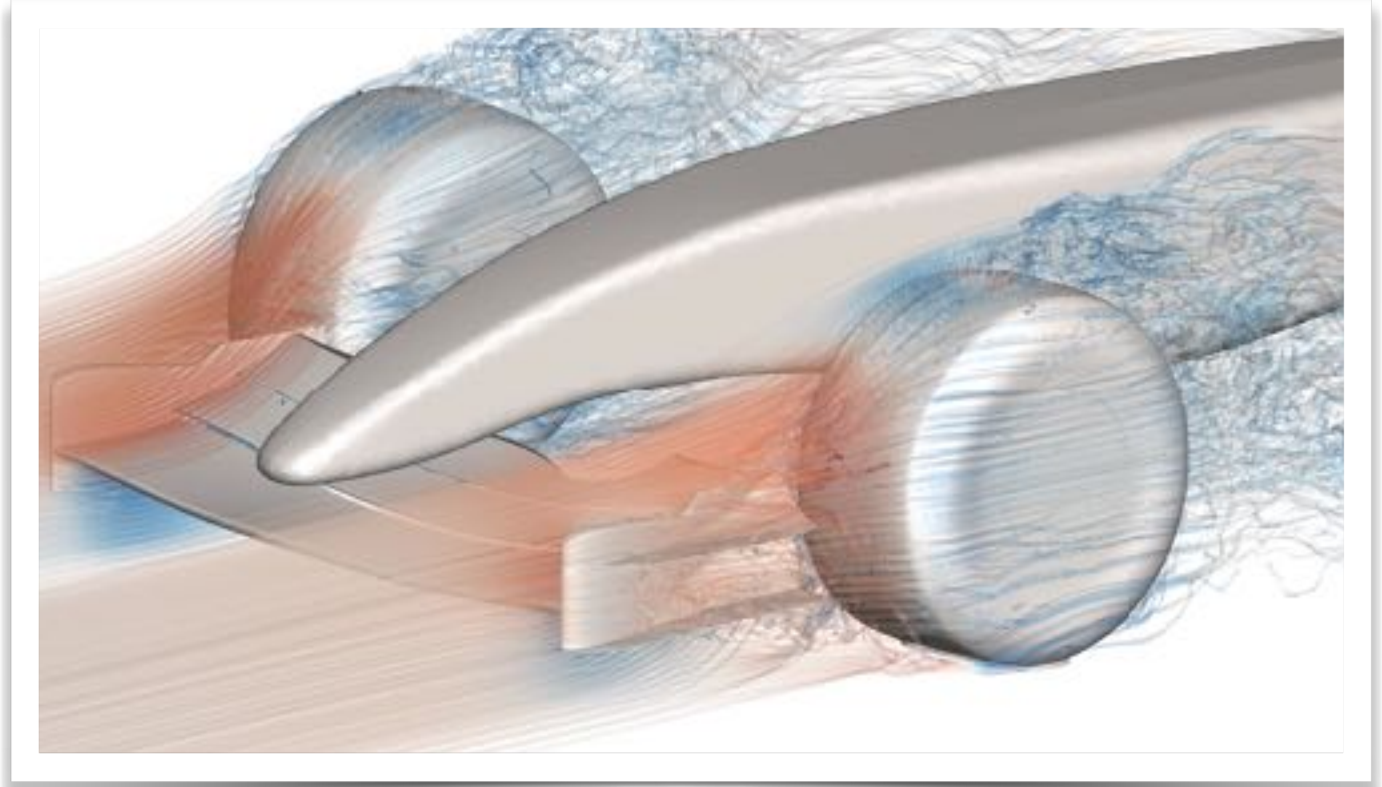
Applications in aeronautics



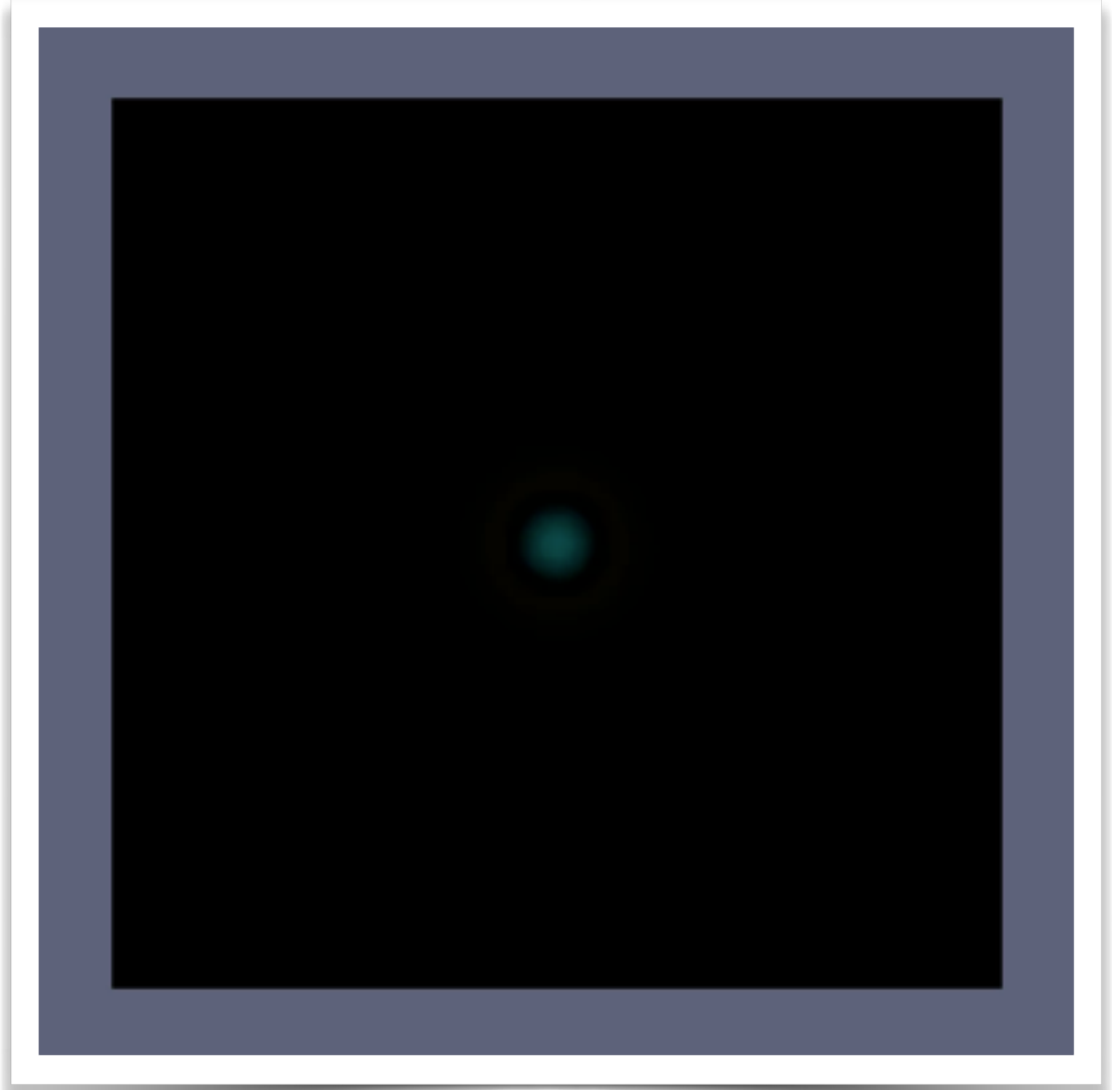
Wavy wing (Serson)



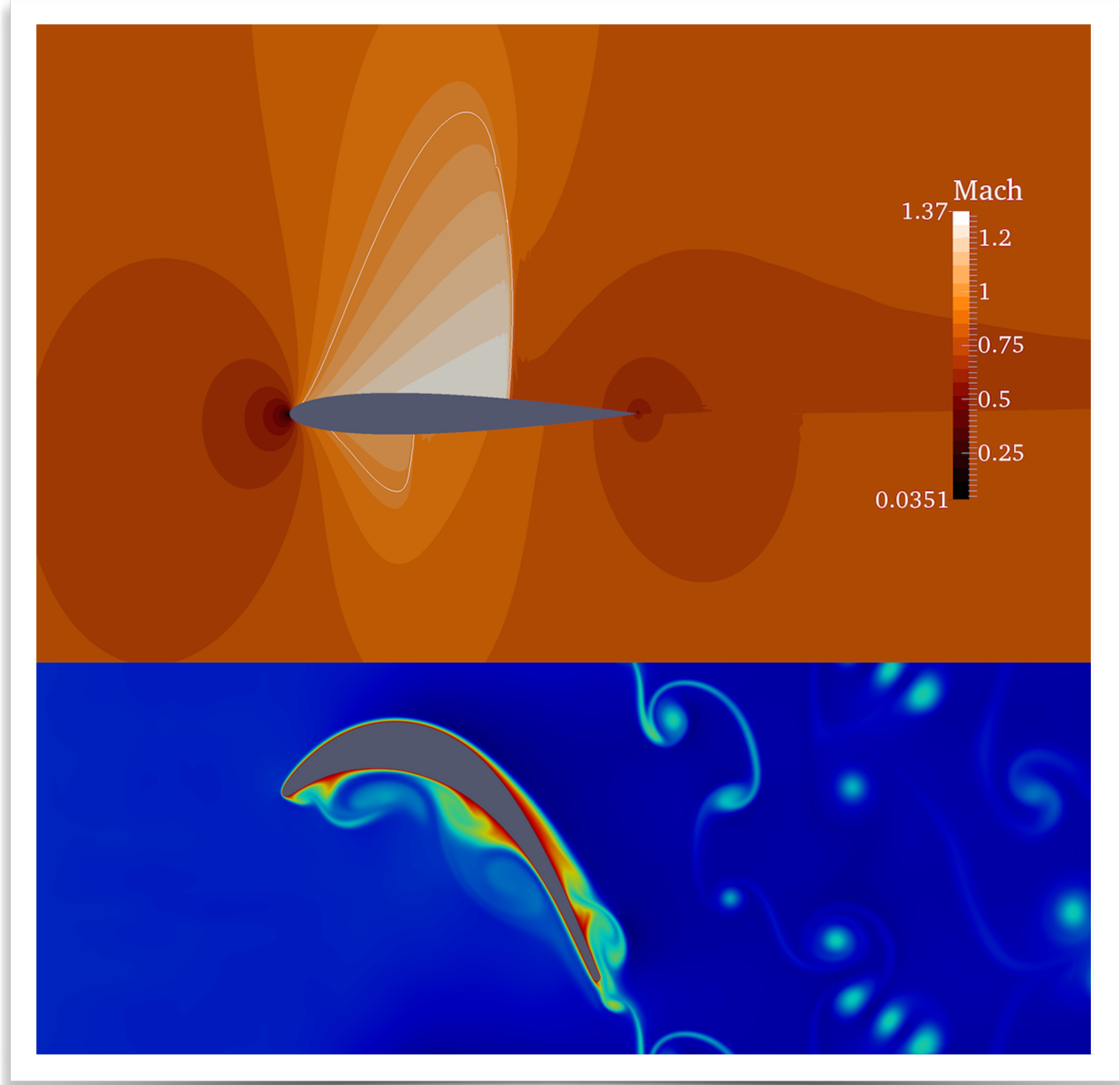
Transition to turbulence (Xu)



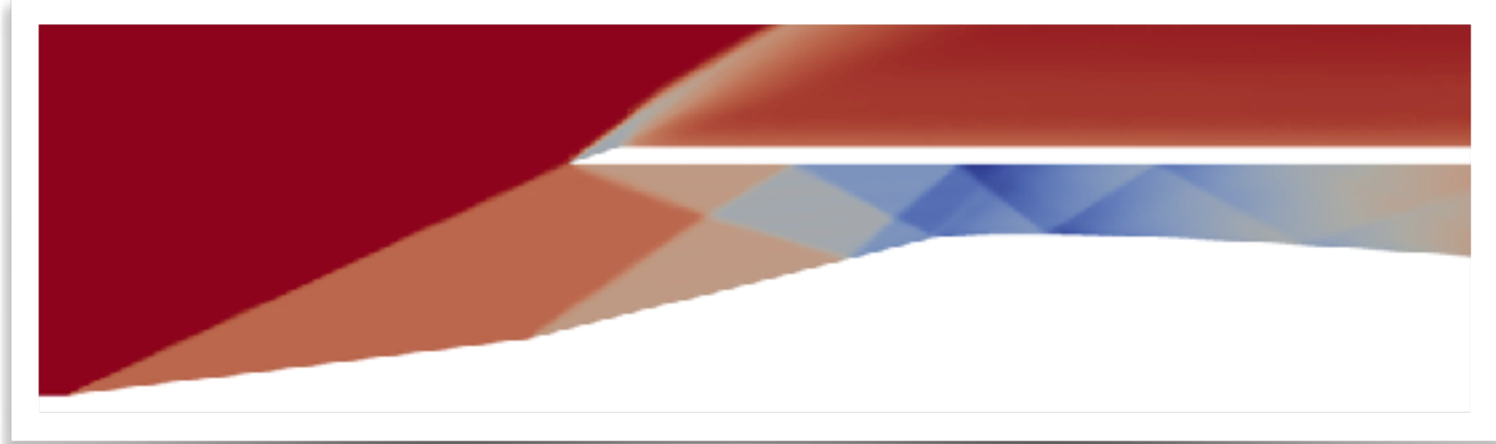
F1 (Lombard, Moxey, Sherwin)

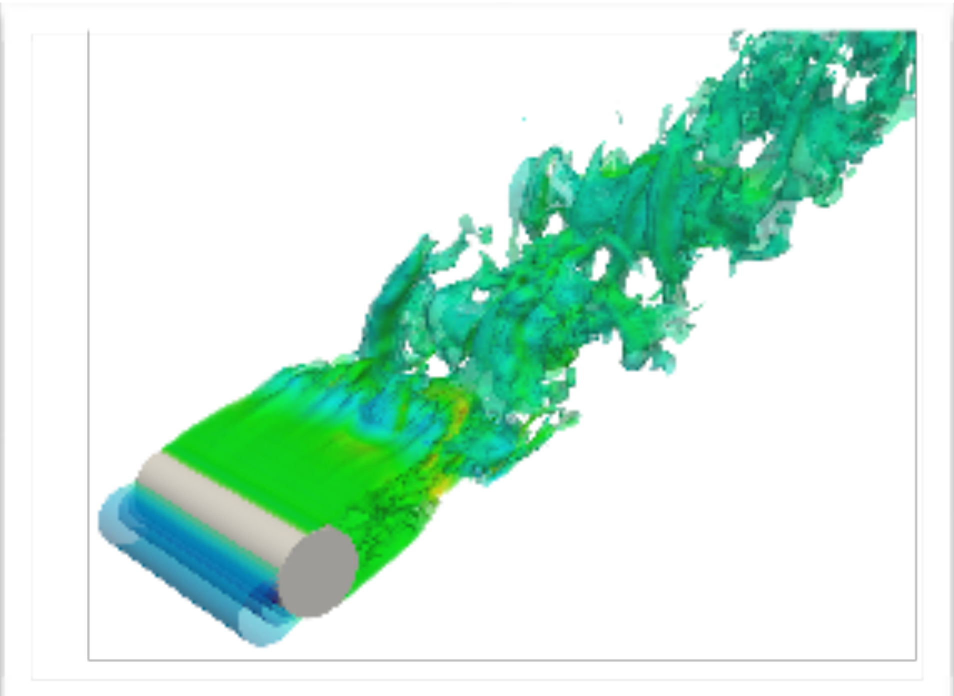


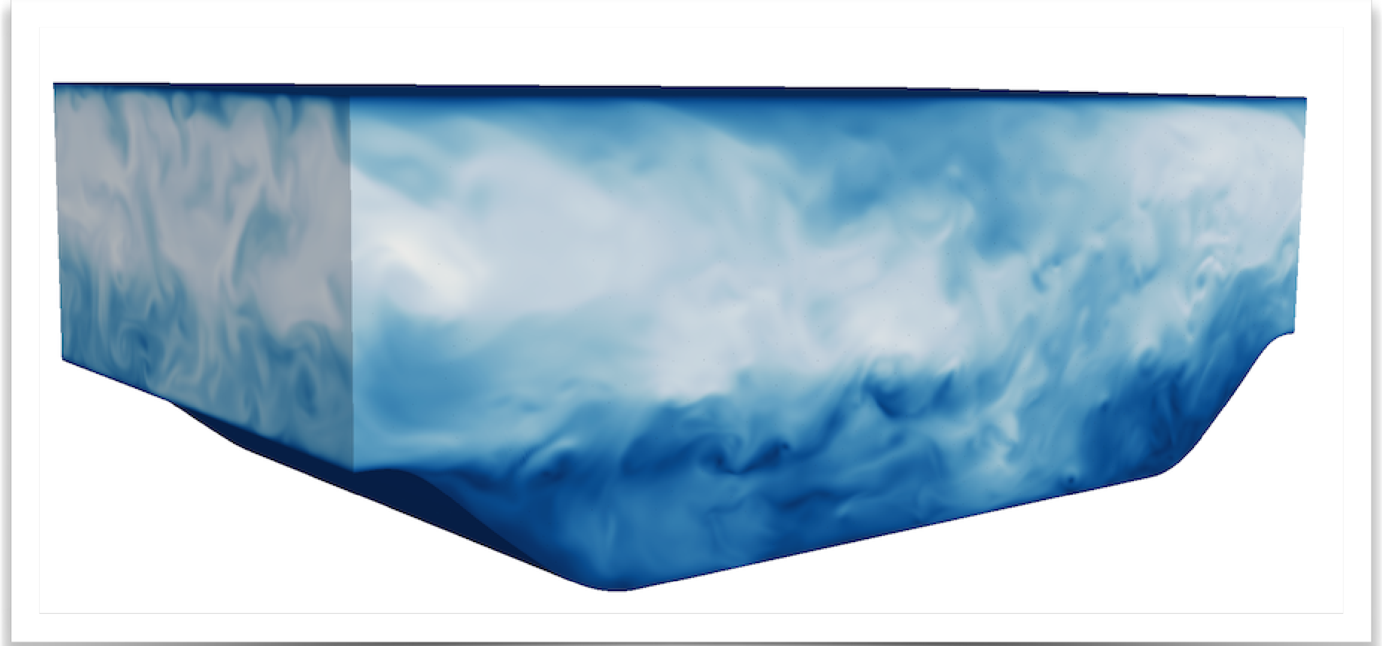
Magnetic turbulence (Moxey)



Compressible flows (Yan, Pan, Mengaldo, Sherwin, Moxey)







Turbulent hill (Moxey)

Moving to problems outside of fluids

- Original spectral/hp implementation for fluid dynamics was made ~20 years ago in a code called Nektar.

- We wanted to expand these methods to things outside of just fluid dynamics. But there were a lot of problems trying to adapt Nektar for this:

    - × No central version control: everyone had their own versions.

    - × No testing: no way to know if code changes/new features broke things.

    - × Almost impossible to generalise to other numerical methods, or physical areas: really was tied to fluids & hard to make work outside of this.

- Motto of the story: it's not enough to write working software: you need to write *maintainable* software. Modern development practices are essential.

Nektar++

spectral/hp element framework

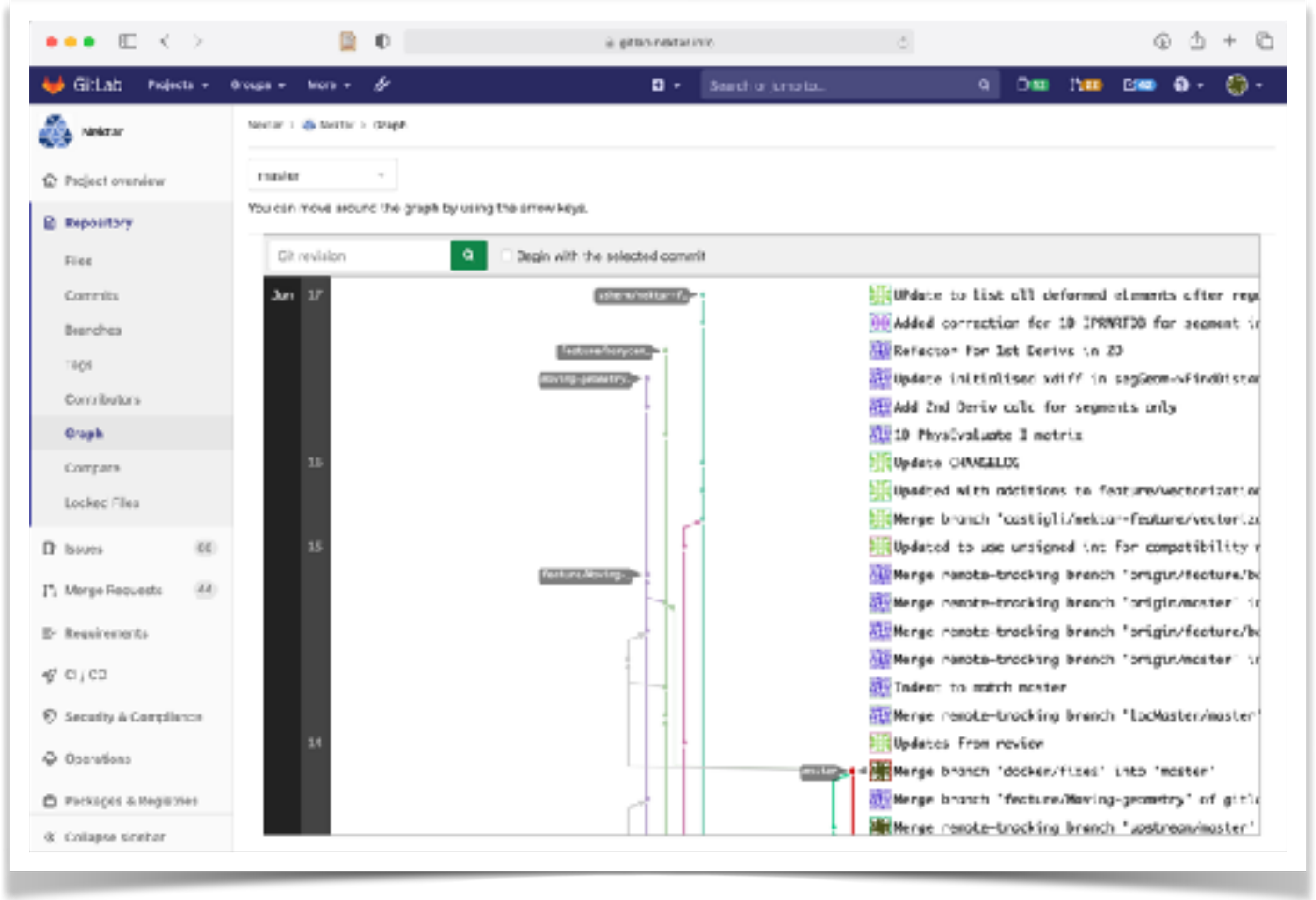
High-fidelity numerical methods
Highly parallel, designed for unsteady flows

Nektar++

spectral/hp element framework

- Nektar++ is an **open source framework** for high-order methods.
- Although fluids is a key application area, we try to make it easier to use these methods in many areas, **not just fluids**.
- C++ API, with ambitions to bridge current and future hardware diversity (e.g. many-core processors, GPUs).
- Runs at lots of scales, from desktops (1-128 cores) through to supercomputers (100k+). Uses pure MPI for parallelisation.
- Modern development practices with continuous integration, git, etc.

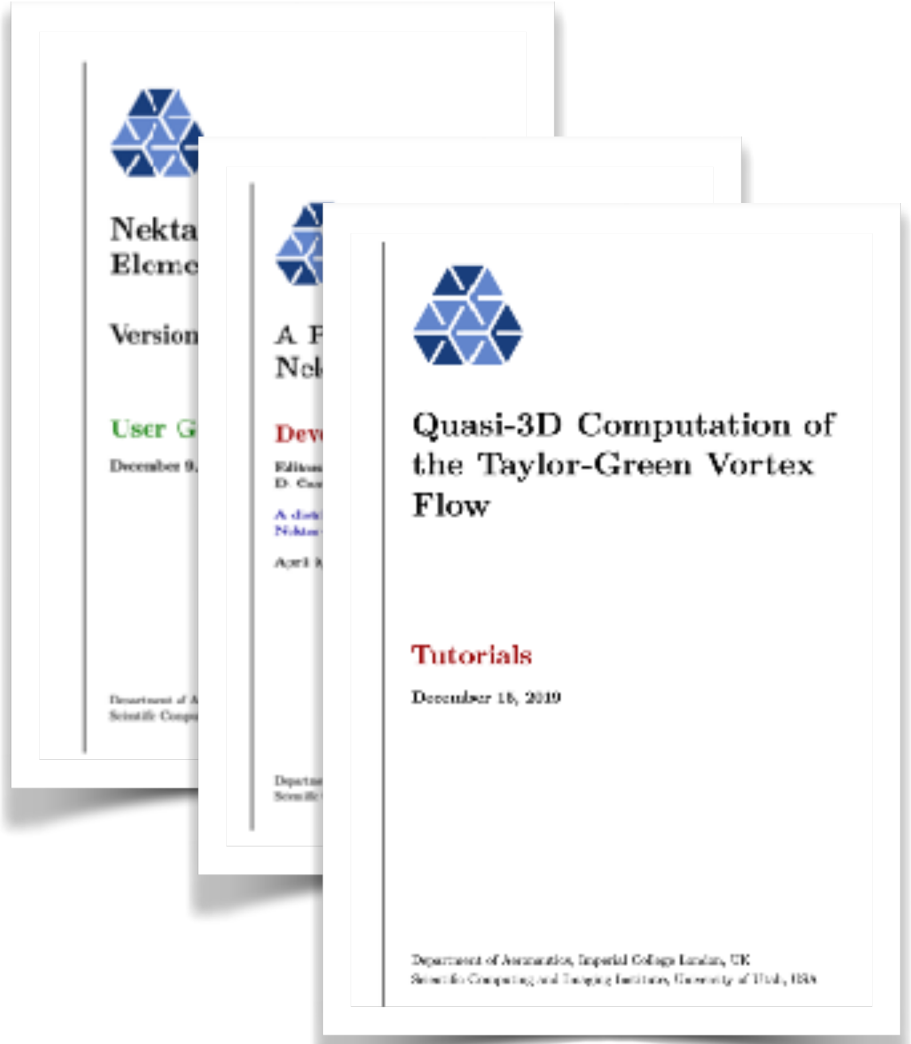
What practices do we use in Nektar++?



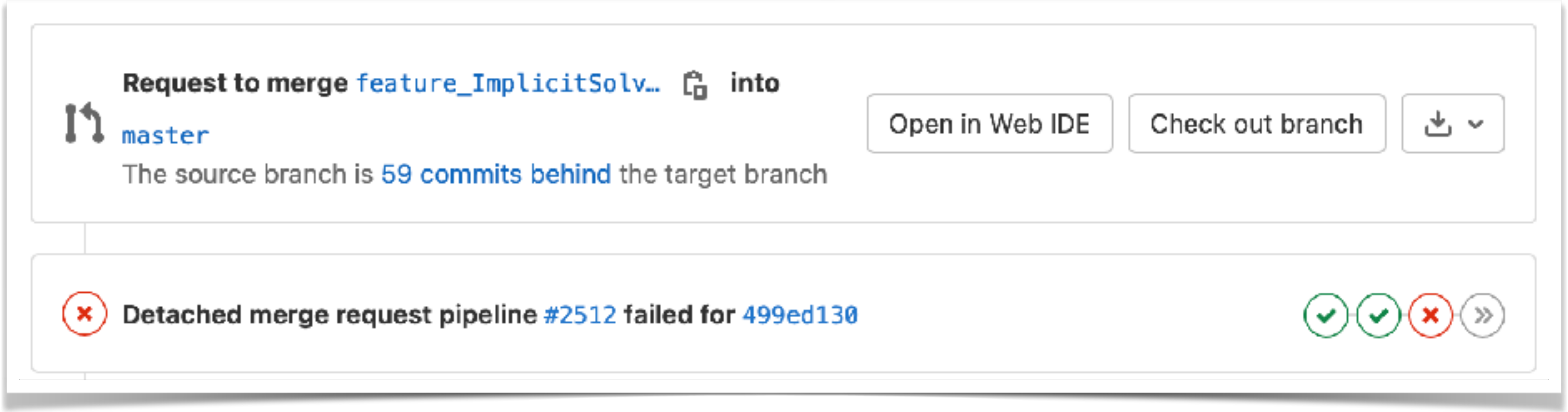
git (hosted on gitlab) for version control

```
docker pull nektarpp/nektar          # binaries
docker pull nektarpp/nektar-dev      # dev image
docker pull nektarpp/nektar-workbook # jupyter
```

docker for containerised builds



documentation + tutorials



gitlab CI for continual integration (testing)

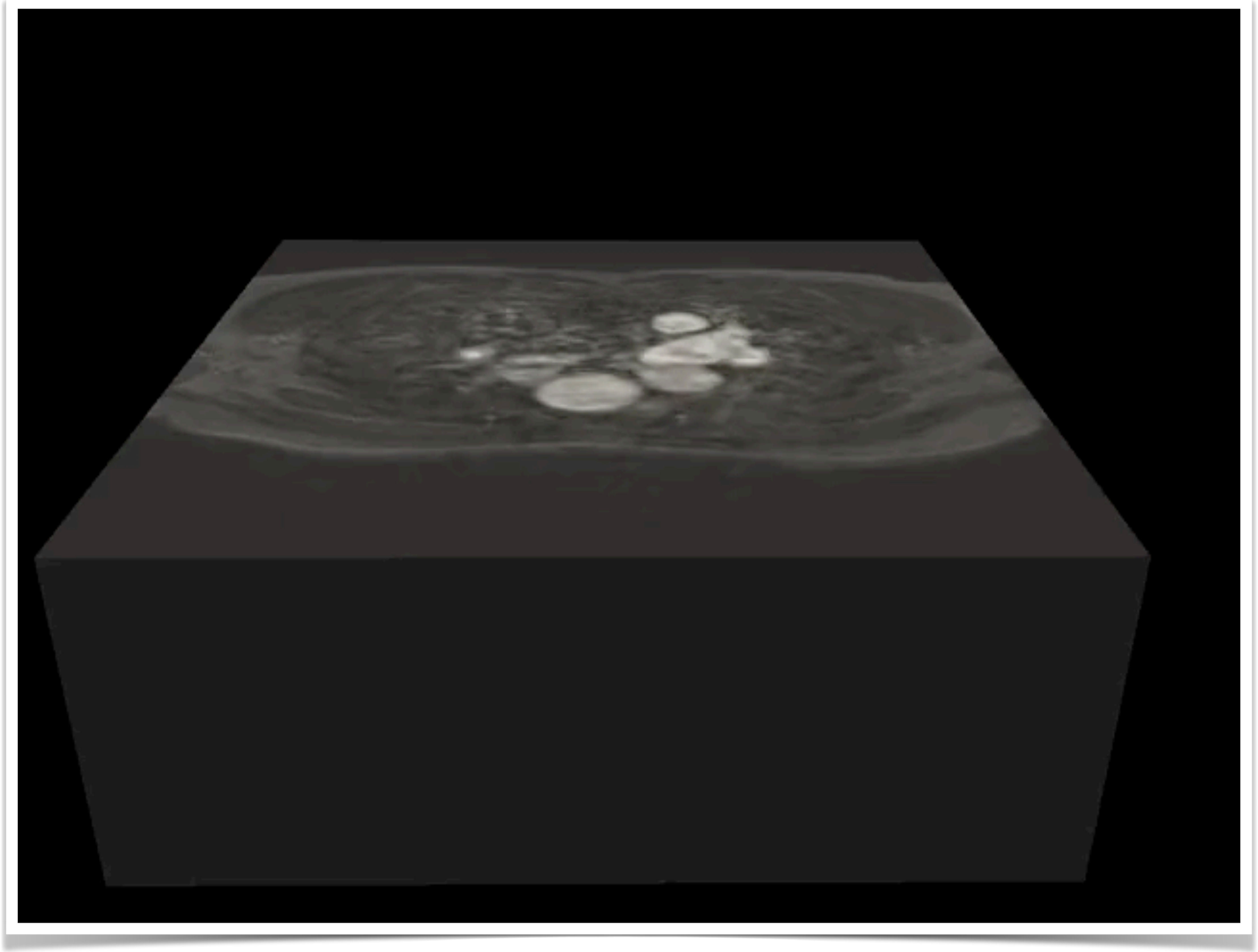
Working on pre-built binaries using continuous delivery: easier installs and releases

What does this give us?

- **Testing + code review:** Allows control over the source, make sure that before new features or fixes are merged, we aren't introducing *new* problems.
- **Docker:** generates an image of the code at each new commit.
  - ✓ Reproducibility is much easier.
  - ✓ Anyone can pull up-to-date master without compiling.
  - ✓ CI built on top of this means we can quickly pull images where things fail and investigate without recompiling.
- **Documentation:** Hopefully easier for people to get started with a complex codebase!
- Properly designed software means we can **extend outside of fluids!**

Modelling cardiac electrophysiology

- Cardiac electrophysiology is the study of how electrical activity occurs in the heart.
- Improve our mechanistic understanding.
  - Examine phenomena in controlled environments.
  - Ask questions which cannot be (easily) tested biologically.
  - Conduct experiments which cannot be (ethically) be performed in vivo.
- Develop emerging clinical tools.
  - Enrich existing clinical mapping technologies.
  - Precision diagnosis.
  - Personalised treatement.

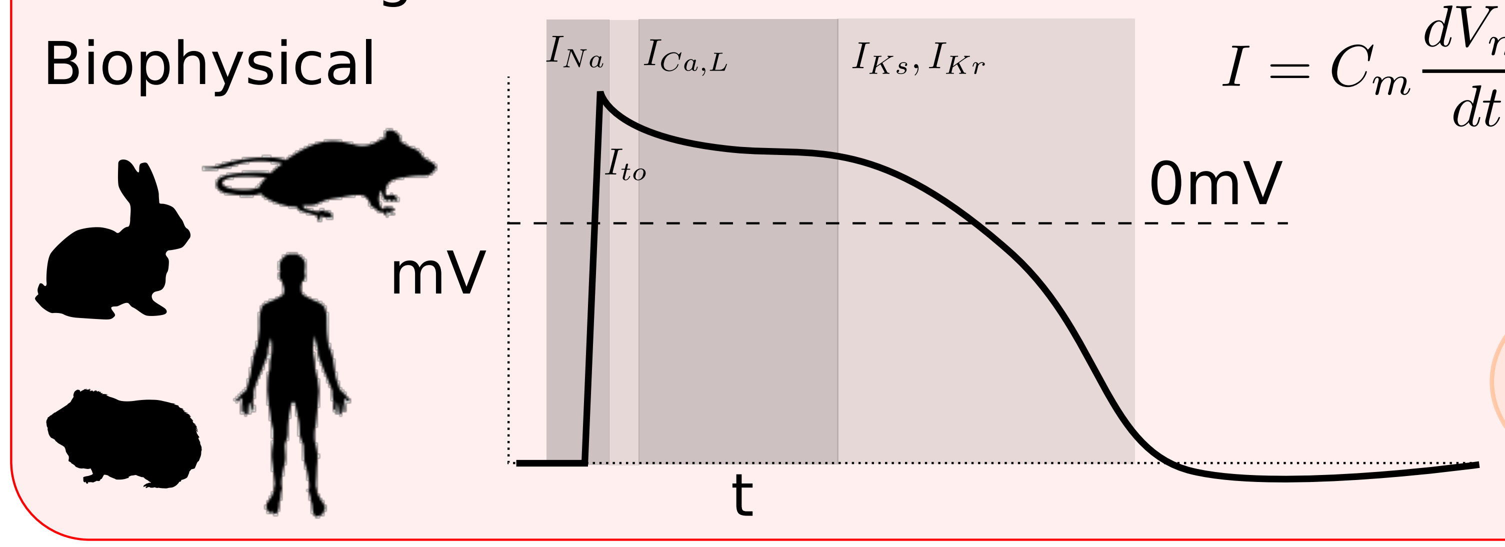


Models for cardiac electrophysiology

Cellular Models of the Action Potential

Phenomenological

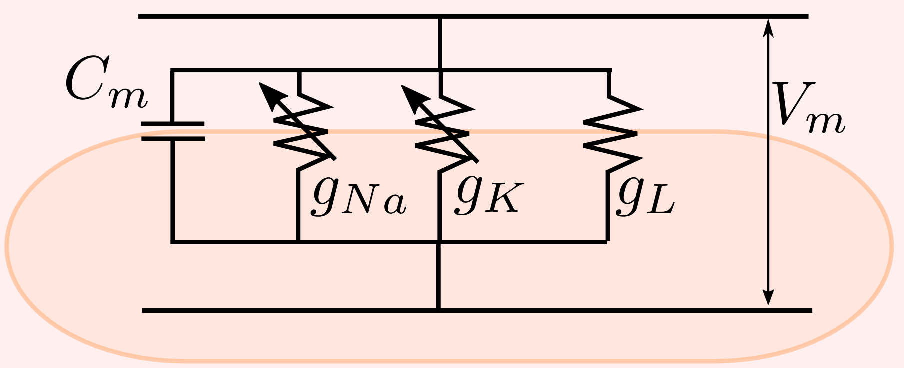
Biophysical



$$\frac{dm}{dt} = \alpha_m(V_m)(1-m) - \beta_m(V_m)m$$

Hodgkin-Huxley

$$I = C_m \frac{dV_m}{dt} + g_{Na} m^3 h (V_m - V_{Na}) + g_K n^4 (V_m - V_K) + g_l (V_m - V_l)$$



Stochastic

Derive models for individual cells

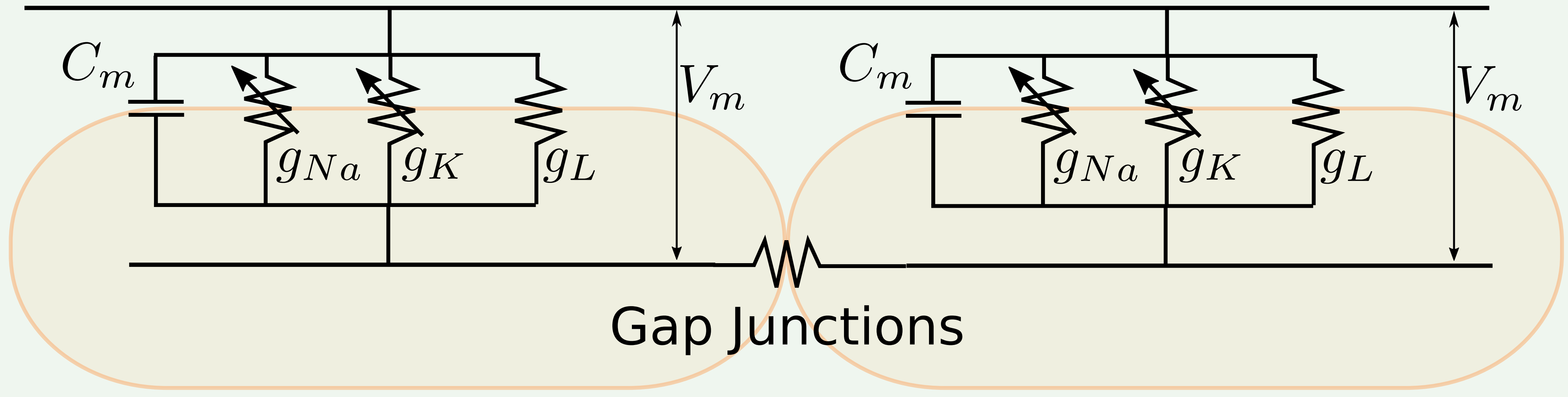
Monodomain Tissue Model

Assumption: $\mathbf{D}_e = \lambda \mathbf{D}_i$

$$\beta \left(C_m \frac{\partial V_m}{\partial t} + I_{ion} \right) = \nabla \cdot \mathbf{D} \nabla V_m$$

...which can be simplified (in some cases)

Inter-cellular coupling

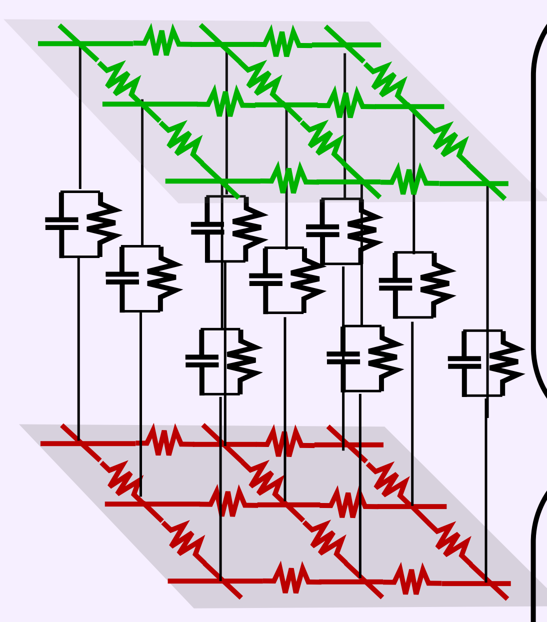


Cells coupled through gap junctions ...however too many of them, so homogenize

Bidomain Tissue Model

$$V_m = V_i - V_e$$

Extracellular



Intracellular

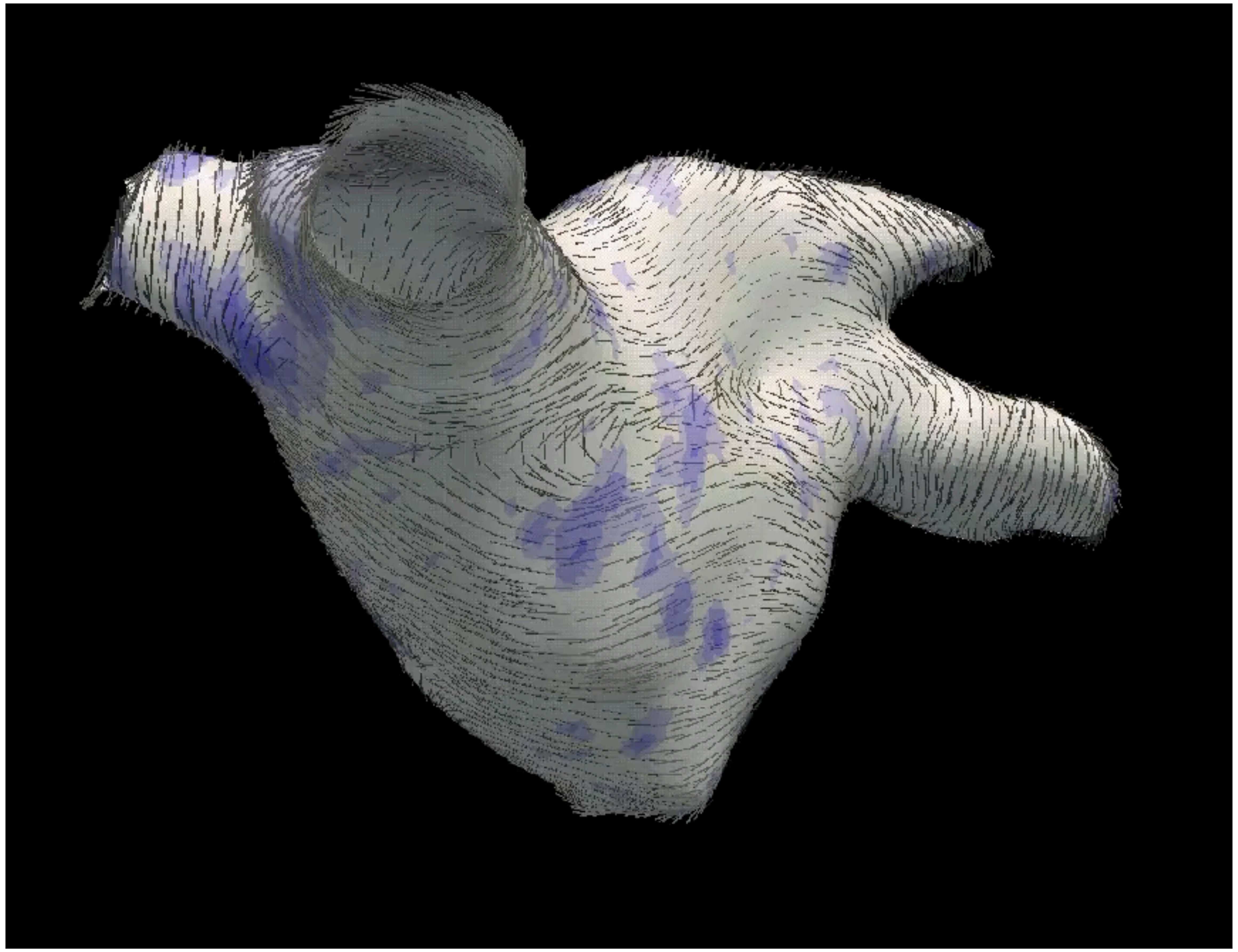
$$\nabla \cdot D_i \nabla V_m + \nabla \cdot D_e \nabla V_e = \beta \left(C_m \frac{\partial V_m}{\partial t} + I_{ion} \right)$$

$$\nabla \cdot D_i \nabla V_i + \nabla \cdot (D_e) \nabla V_e = 0$$

Leads to a PDE

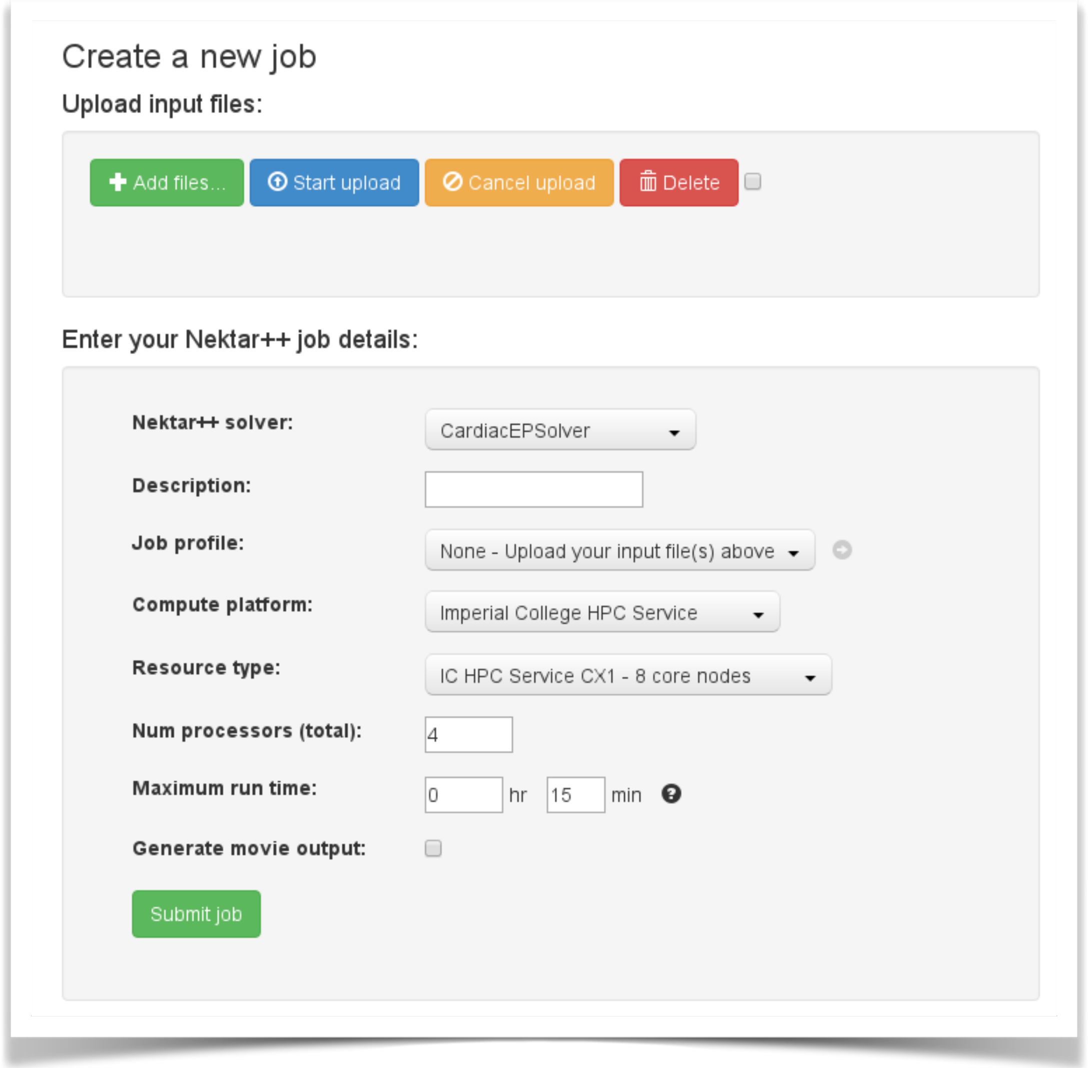
Personalised models

- Great potential in computational modelling for *personalised* models to tailor treatment for specific patients.
- Incorporate multi-model clinical data:
  - ➡ Imaging (MR/CT)
    - Chamber geometry
    - Location of scar (LGE-CMRI)
  - ➡ Electroanatomic mapping
    - Activation patterns
    - Nature of arrhythmia
- Use these to tailor simulation parameters (e.g. diffusion tensor), understand how different treatments may affect activation patterns.

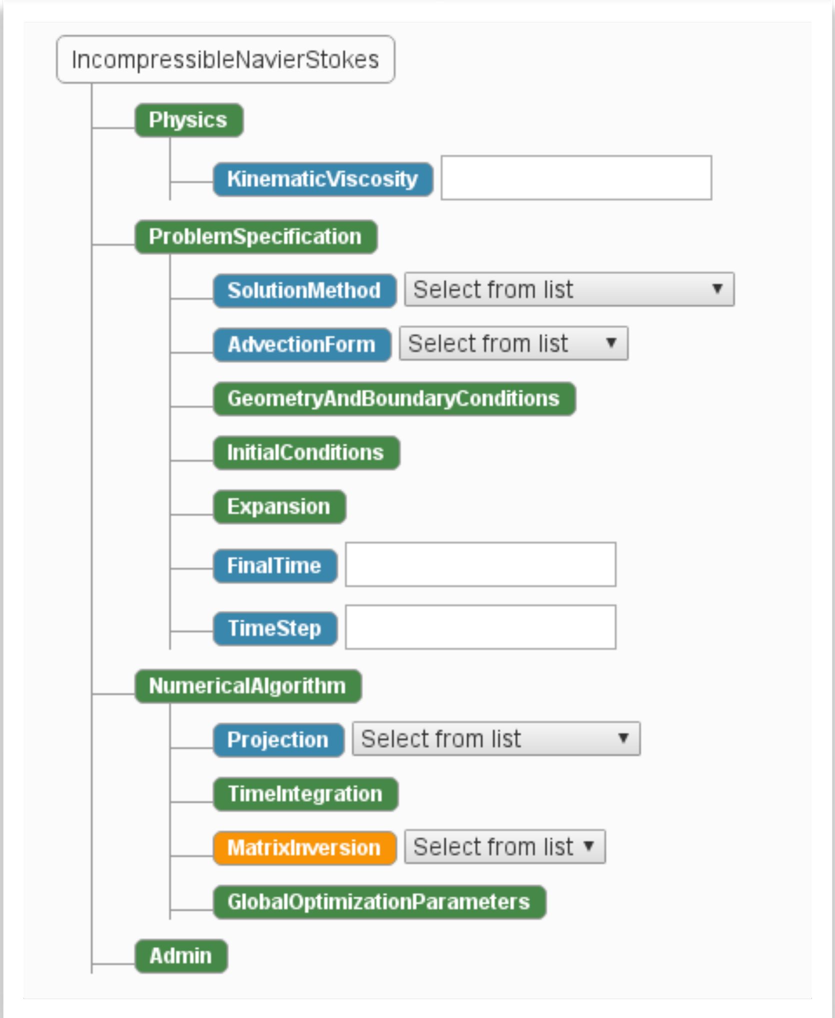


More on software: increasing usability

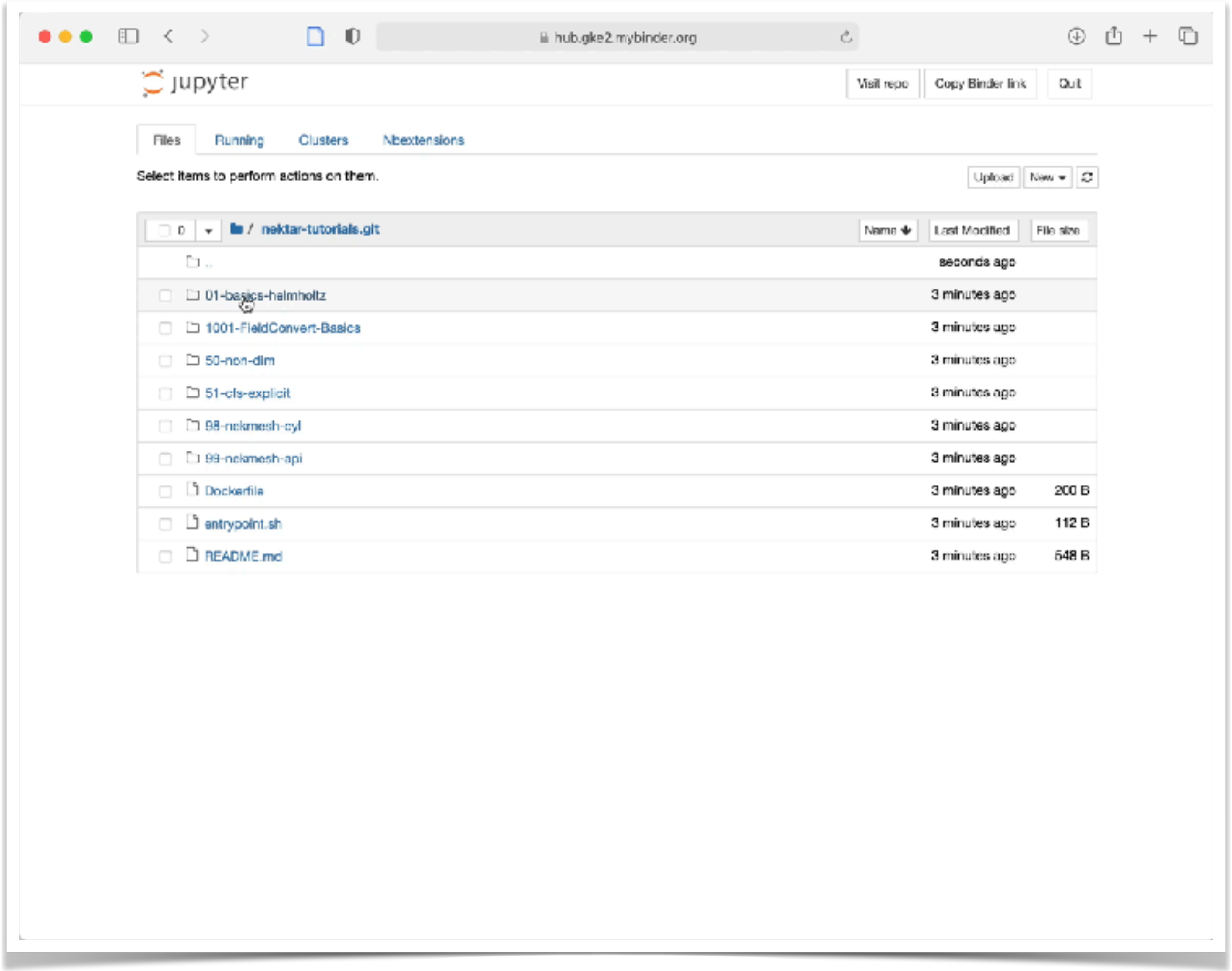
- Software like Nektar++ is increasingly complex to use & configure.
- Working on several approaches to reduce complexity for end-users & clinicians.



Nekkloud
web-based simulations
backed by cloud resources



TemPSS
web-based configuration
enables constraints/validation



Jupyter
Running simulation in-browser

Summary

- Combination of cutting-edge models and high-quality software can give deep insights into challenging problems: from increasing downforce to understanding life-altering diseases.

- Learning about research software development and how to effectively use modern practices can be hugely beneficial.

- Lots of challenges still to overcome!

    - How do we make tools easier to set up and use?

    - How do we deal with the wealth of parameters, meshing, etc?

    - How do we do a better job of handling uncertainty?

Thanks for listening!

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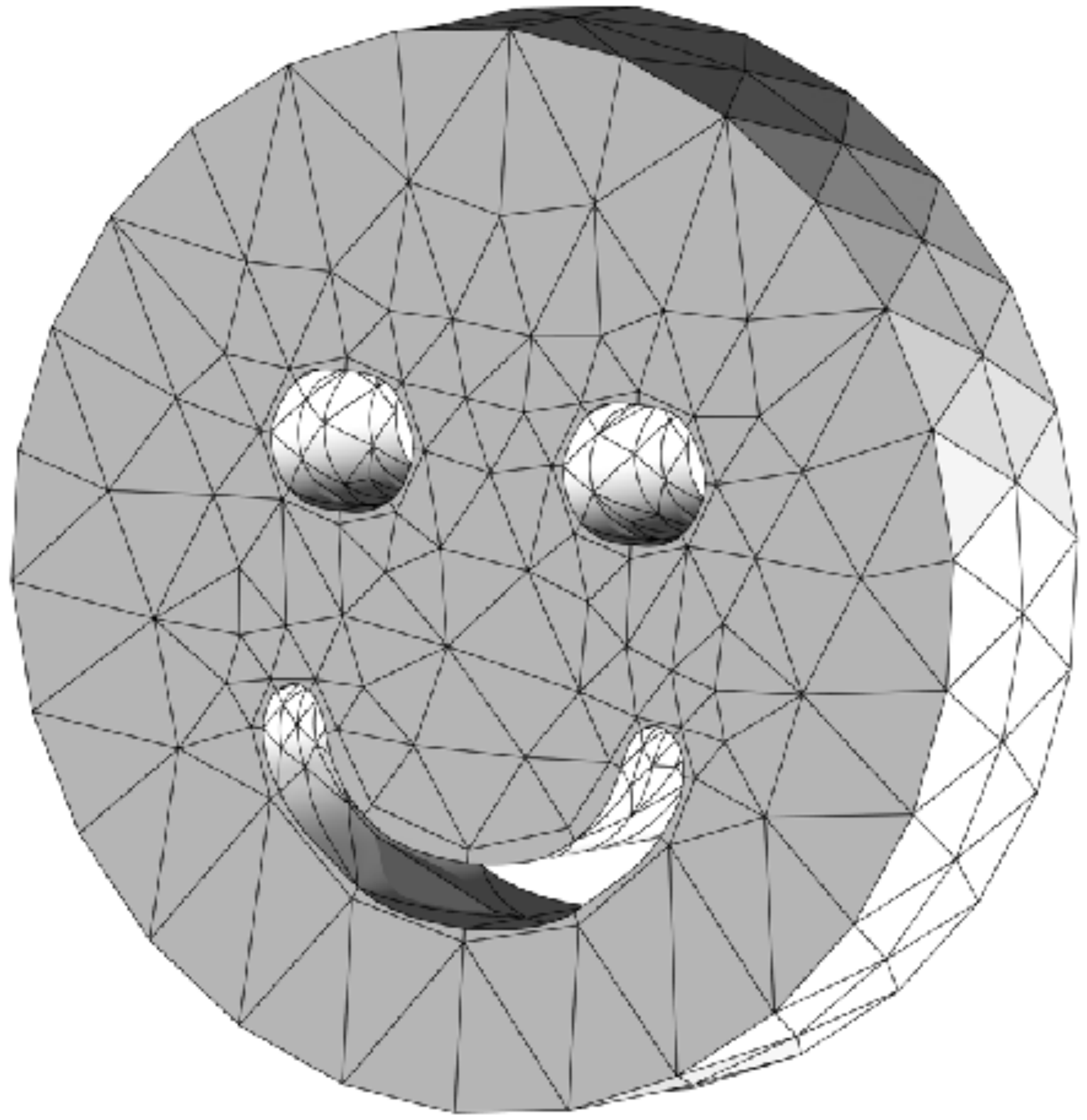
https://prism.ac.uk/



EPSRC

Pioneering research and skills

Nektar++: enhancing the capability and application of high-fidelity spectral/*hp* element methods

David Moxey[1], Chris D. Cantwell[2], Yan Bao[3], Andrea Cassinelli[2], Giacomo Castiglioni[2], Sehun Chun[4], Emilia Juda[2], Ehsan Kazemi[4], Kilian Lackhove[6], Julian Marcon[2], Gianmarco Mengaldo[7], Douglas Serson[2], Michael Turner[2], Hui Xu[5,2], Joaquim Peiró[2], Robert M. Kirby[8], Spencer J. Sherwin[2]