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Translating high order spectral/hp element methods from academia to industry

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Journey from Academia to Applications

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Long



Imperial College Spectral/hp element Methods ELEMENT London spectral methods $U_{\delta} = \{$ $U_{\delta} =$ finite difference Spectral/hp methods finite element/finite volume $U_{\delta} = \{$

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Spectral/hp elements





Computational cost ~ P4 Computational error ~ h^p

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Scales of CFD



uDNS/iLES



RANS

DES



Moxey, Turner, Peiro, Jassim, Taylor, Sherwin Design 3: +270% Downforce

High-order mesh generation



Pre analysis stage in FE simulations

- Preparation of CAD models for mesh generation is still the major bottleneck.
- This is estimated to take about 80% of the time invested in an analysis.
- Mesh generation algorithms require water tight geometries.

Cleaning

• Very small curves and surfaces that will cause excessive mesh refinement

De-featuring

 Dealing with complex objects that contains multi-scale features it is often necessary to manually remove small features

Courtesy of Oubay Hassan, Swansea University









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Boundary layer meshing

Meshing



High-order mesh generation

- Starting point is typically a linear mesh
 - Have large elements or smaller meshes for a given volume
 - For complex geometries we still require to larger meshes to capture relevant features.
- In-situ adaptation could be useful.
 - Require access to geometry representation/CAD



Meshing Pipeline



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Nektar++ Stack







Post processing

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- •5GB data files per time snapshot.
- Post processed on 24 core node
- Domain decomposition into 100 partitions
- In-house iso-contour extraction to process each partition in task based manner
- Batch processed snapshot through vis package to get jpg file and then constructed movie
- Clearly a number of sub-steps to decide on isocontour, view angle etc!
- •Data set movement becoming challenging
- •On site post-processing
- In-situ processing
 - •Similar to experimental campaigns where we need to decide on data capture
 - Likely to require interactive adjustment

- Can use library to setup post-processing call from input file
- Have developed python interface to modules

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Maintaining Code Stability

Development practices & Software Engineering

- Version-control (Git + Gitlab)
- Tests & Continuous Integration (Gitlab CI)

• Issue tracking (Gitlab)

•gitlab.nektar.info

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Active Development Team: Senior Developers

ELEMENT

- Already requires CAD preprocessing/De-featuring
- Also need appropriate format, i.e. hdf5
- In-situ analysis increasingly required
 - Interactively steer analysis.
- Software: Maintainability and evolution of code is possible since we have original development team.
 - •What is process for legacy or community codes without development team?

1.What do you see as the key challenges Exascale presents from an end-user point of view?

2.Based on the presentations what aspects of pre- and post-processing for Exascale computing have not been covered? Note that Geometry, CAD and Adaptivity are to be discussed in the next session.

3.What are the plans for essential legacy codes and how to engage with Exascale systems over the next decade? For example: establish new development groups, develop middleware for pre- and post-processing, move to other code-bases, hope for the best ...