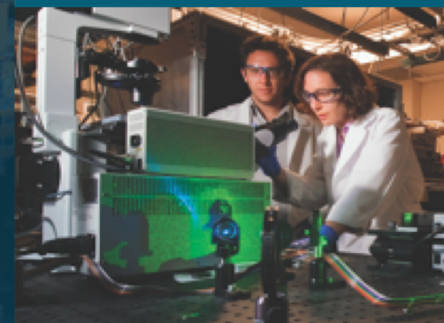
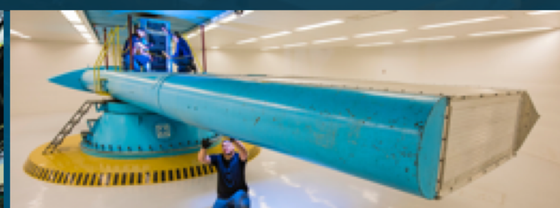
Guest Lecture Stanford ME469: Common low-Mach Discretization Approaches





PRESENTED BY

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Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND2018-4536 PE

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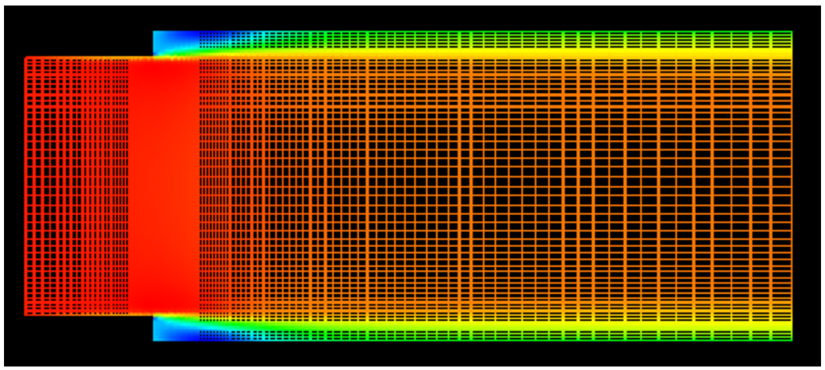
Common low-Mach Discretization Approaches: Outline

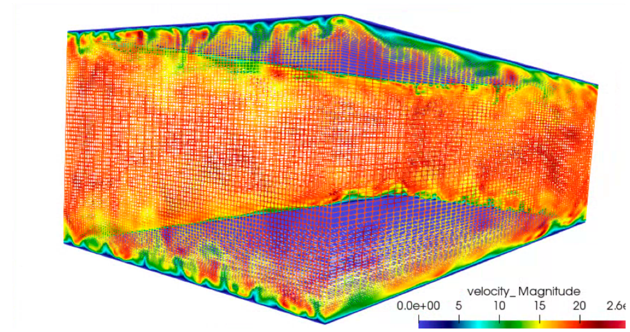
- Why Unstructured?
- Unstructured Element Typoes
- Model PDE for Discretization
- Finite Element Method (FEM)
- Control-Volume Finite Element Method (CVFEM)
- Edge-based Vertex-Centered (EBVC)
- Cell-centered Finite Volume (FV)
- Staggered arrangement
- Conclusions

Structured vs Unstructured

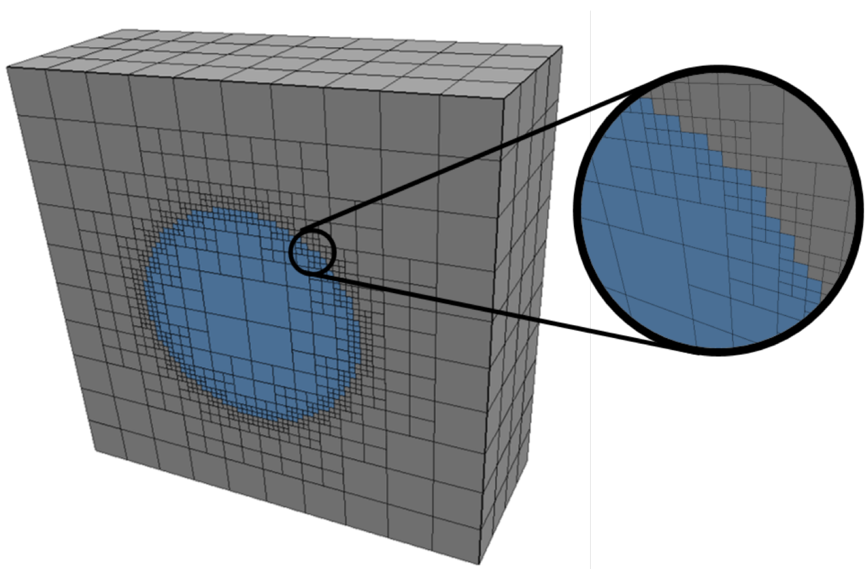
- Many times, the canonical flows of interest are in simplified geometries that allow for cartesian meshes – with "stair-stepping"

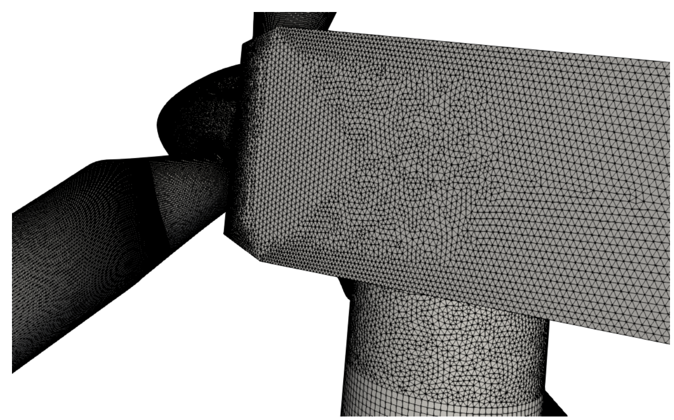


RANS-based backward facing step (Domino, 2012)



Re_τ 395 plane-channel (Jofre, Domino, Iaccarino, 2018)



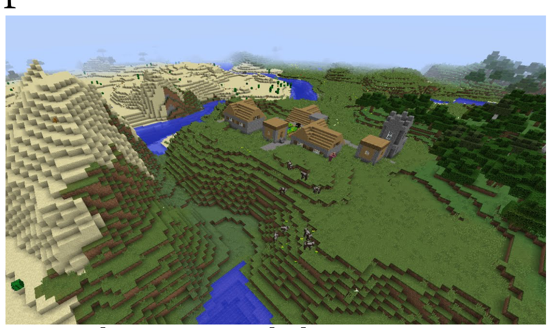


Often times, not!

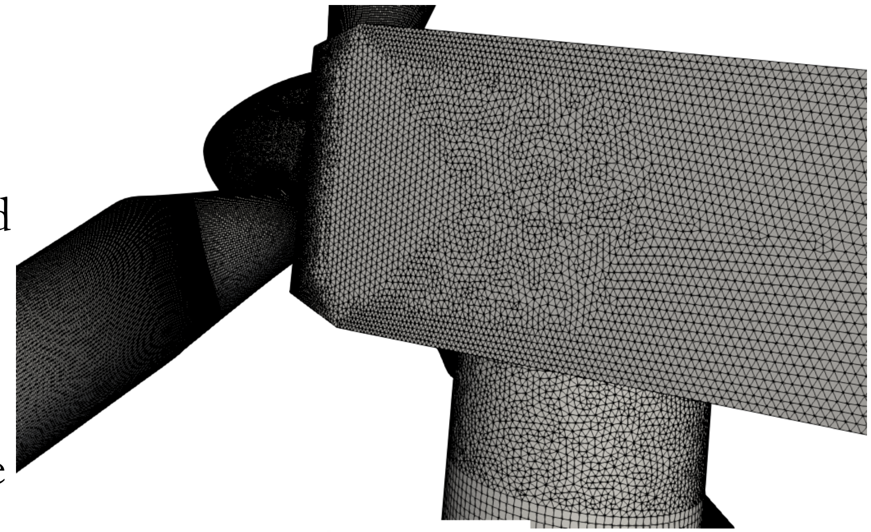
https://www.itascainternational.com/software/introduction-to-meshing

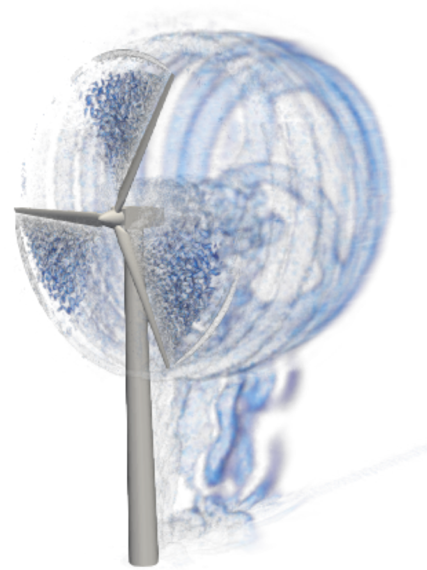
Reality: Meshing time for complex applications remains a significant bottleneck!

- Many applications of interest to SNL contain complex geometries
- low-Mach fluids users interested in high-quality simulation results tend towards hexahedral-based topologies (if possible)
- However, if a scheme is "design-order" accurate, any topology may suffice as it is simply a matter of mesh size and efficiency – not unlike the active discussion on low- vs higher-order
- Sometimes, the penetration of a low-Mach fluids physics addition in common analysis is high as the meshing can be prohibitively complex



Very complex world – stair-stepped!

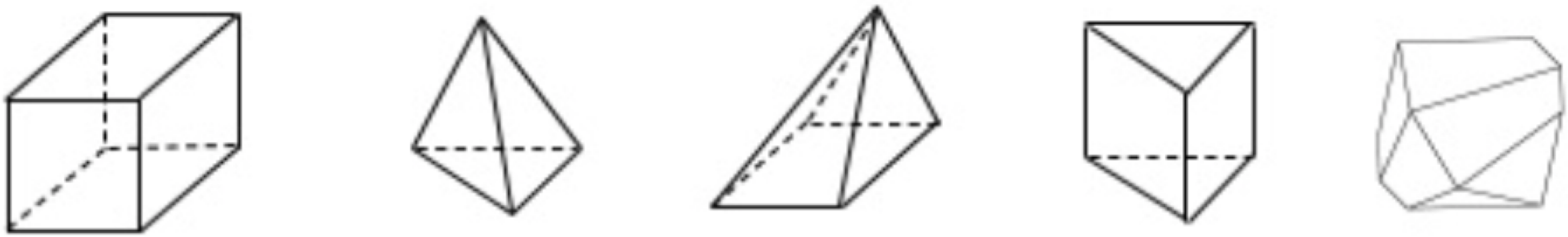


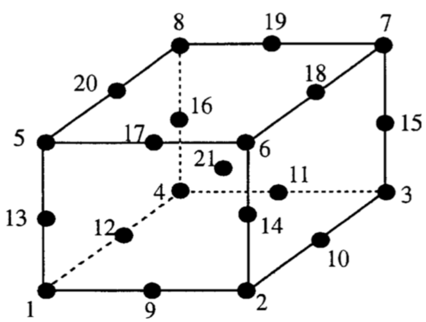


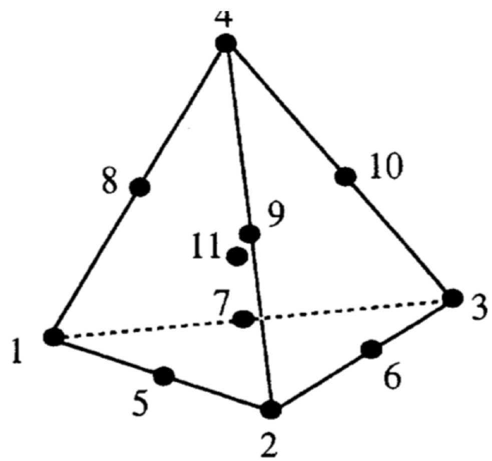
UUR Example: Vestas V27 225 kw hybrid low-order hex/tet/pyr/wedge

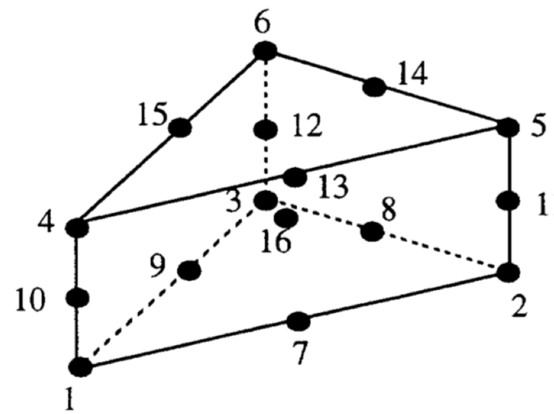
Examples of Various Topologies

Hex8 | Tet4 | Pyramid5 | Wedge6 | Arbitrary



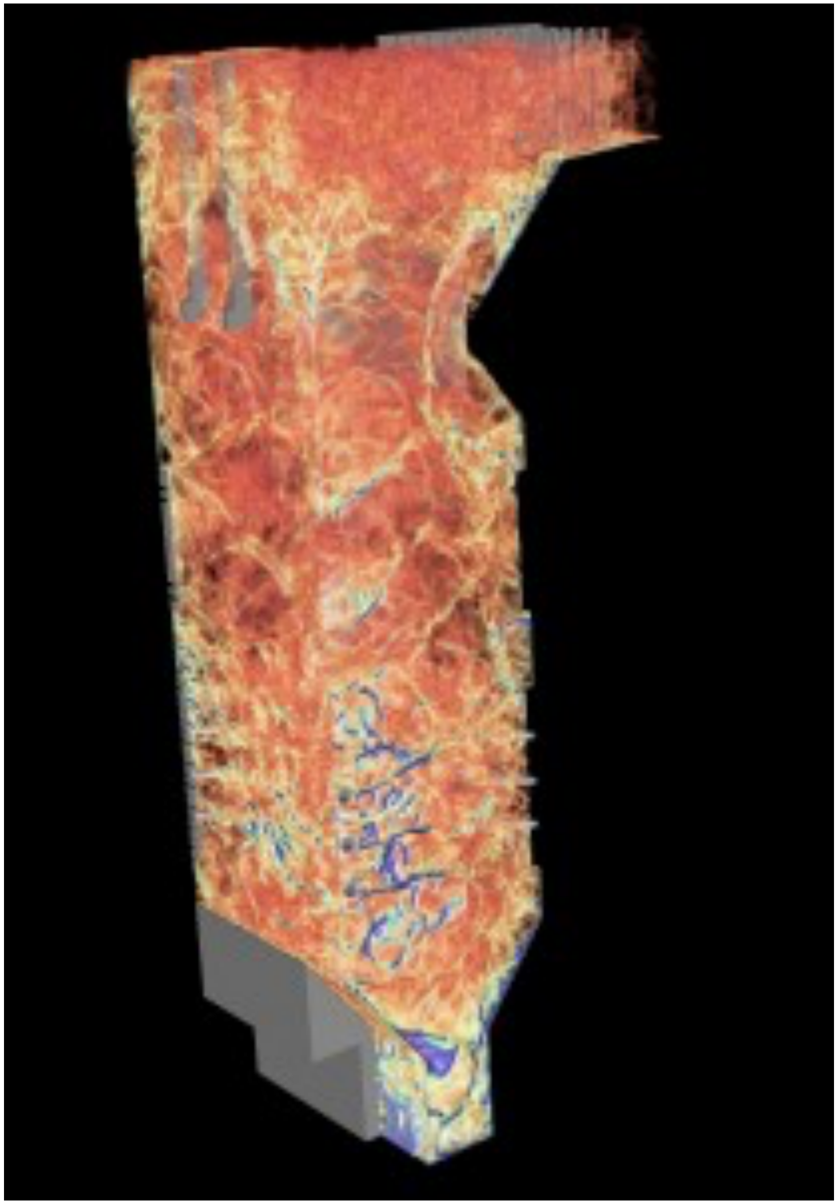






Higher-order promoted elements (Hex27, Tet10, Wedge16, Hex64, etc.)

In Fairness....
The Carbon-Capture Multidisciplinary Simulation Center



http://ccmsc.utah.edu/about.html

15MW coal-fired boiler volume rendered image of large (90 μm) particles

Staggered schemes have been demonstrated to support complex applications

Cut-cells and embedded approaches help

Fundamentals of Discretization

- Given a partial differential equation (PDE) and associated volumetric form:

$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} = 0 \qquad \int \rho C_p \frac{\partial T}{\partial t} dV - \int \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV = 0$$

- Applying Gauss Divergence provides the standard finite volume form:

$$\int \frac{\partial q_j}{\partial x_j} dV = \int q_j n_j \, dS \qquad \int \rho C_p \frac{\partial T}{\partial t} dV - \int \lambda \frac{\partial T}{\partial x_j} n_j \, dS = 0$$

- We can also multiple PDE by an arbitrary test function, w, and integrate over a volume,

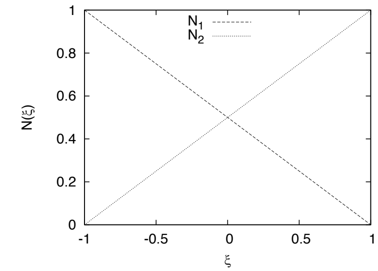
$$\int w \rho C_p \frac{\partial T}{\partial t} dV - \int w \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} n_j \, dS = 0$$

Next, integrate by parts and apply Gauss-Divergence:

$$\int w \rho C_p \frac{\partial T}{\partial t} dV + \int \frac{\partial w}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV - \int w \lambda \frac{\partial T}{\partial x_j} dS = 0$$

Sometimes, you see T as T^H - the trial space

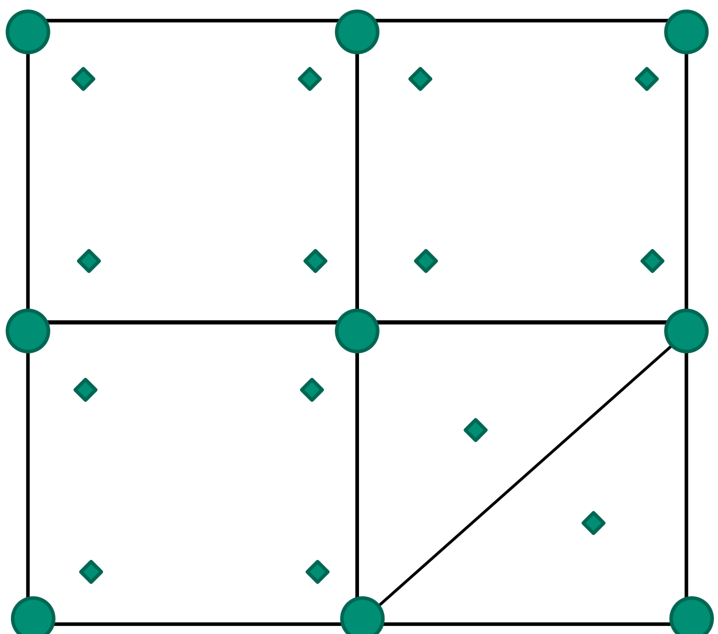
The Finite Element Method (FEM)



- Consider an alternative approach in which a finite element method (FEM) is employed

- Define an underlying nodal basis with the element:

$$T(x_k) \approx \sum_{i=1}^{npe} N_i(x_k) T_i \qquad \frac{\partial T(x_k)}{\partial x_j} \approx \sum_{i=1}^{npe} \frac{\partial N_i(x_k)}{\partial x_j} T_i$$



- Gaussian Quadrature is used

- On a -1:1 range, +/- sqrt(3)/3

- Consider a simple heat conduction model PDE,

$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} = 0$$

- Integrate using a test function,

$$\int w \rho C_p \frac{\partial T}{\partial t} dV - \int w \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV = 0$$

- Integration-by-parts (with G-D) provides:

$$\int w \rho C_p \frac{\partial T}{\partial t} dV + \int \frac{\partial w}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV - \int w \, \lambda \frac{\partial T}{\partial x_j} n_j dS = 0$$

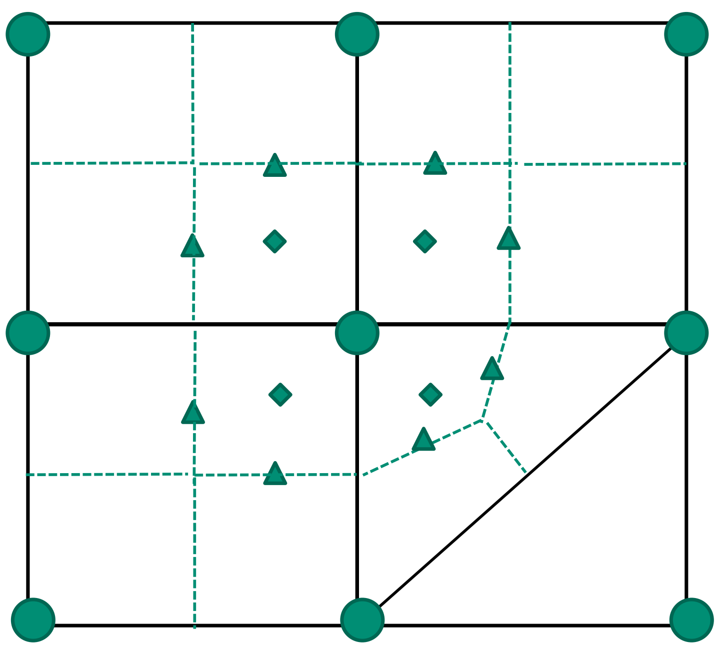
- Iterate element quadrature points

- Note that N can be arbitrary in order (shown here for a linear)

The Hybrid Control-Volume Finite Element Method (CVFEM)

- A combination between the edge-based vertex-centered and FEM is the method known as Control Volume Finite Element ()
- A dual mesh is constructed to obtain flux and volume quadrature locations
- As with FEM, a basis is defined:

$$T(x_k) \approx \sum_{i=1}^{npe} N_i(x_k) T_i \qquad \frac{\partial T(x_k)}{\partial x_j} \approx \sum_{i=1}^{npe} \frac{\partial N_i(x_k)}{\partial x_j} T_i$$



Dual-volume definition

- Integration-by-parts over test function w:

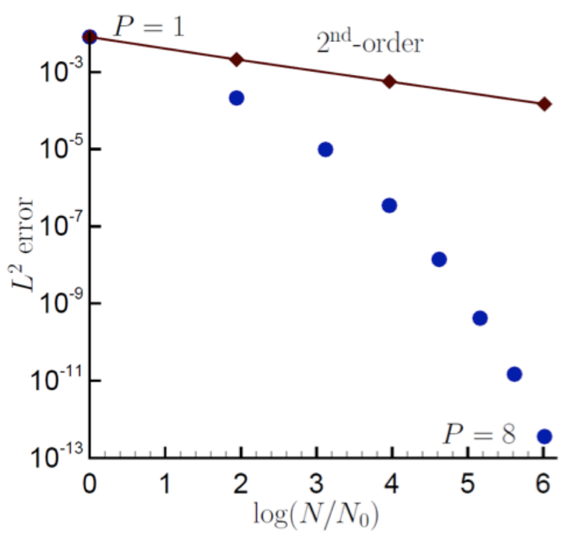
$$\int w \rho C_p \frac{\partial T}{\partial t} dV + \int \frac{\partial w}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV - \int w \, \lambda \frac{\partial T}{\partial x_j} n_j dS = 0$$

- However, define a test function, w, as a piece-wise constant function (Heavyside) to be 1 inside the dual volume and 0 outside. Gradient is a Dirac-delta function: $\frac{\partial w}{\partial x_j} = -n_j \delta(x_j - xIP_j)$

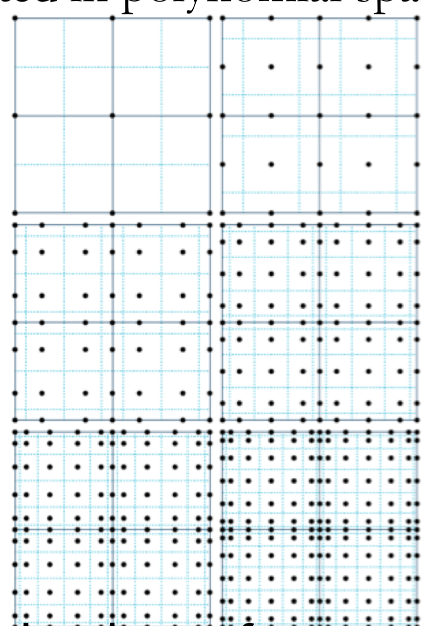
- Leading to: $\int \rho C_p \frac{\partial T}{\partial t} dV - \int \lambda \frac{\partial T}{\partial x_j} n_j \, dS = 0$

Control-Volume Finite Element Method Attributes

- The CVFEM method, therefore, is a finite volume scheme that is locally conservative, i.e., momentum leaving one dual volume face enters the adjacent dual volume
- However, the gradient operator, like its FEM counterpart is absent of any error due to non-orthogonality
- Since the test-function, w, is different from the underlying basis representation, this method can be considered a Petrov-Galerkin method
- The method can also be promoted in polynomial space



Spectral convergence



Dual-volume for promoted quad4

P=1 (left) and P=4 (right) Helium plume (VR-density)

Dual Volume Definitions for Hybrid Meshes

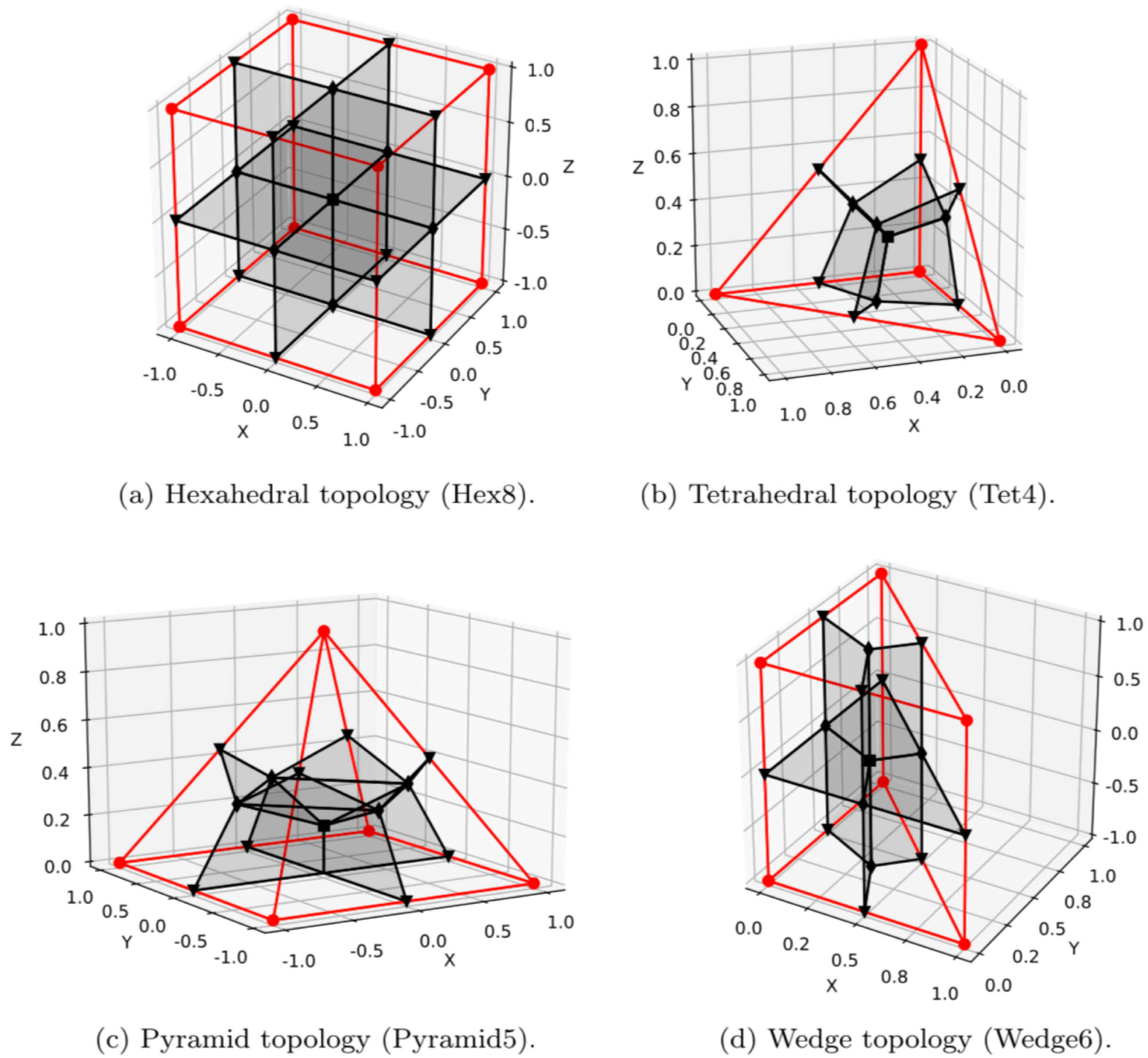
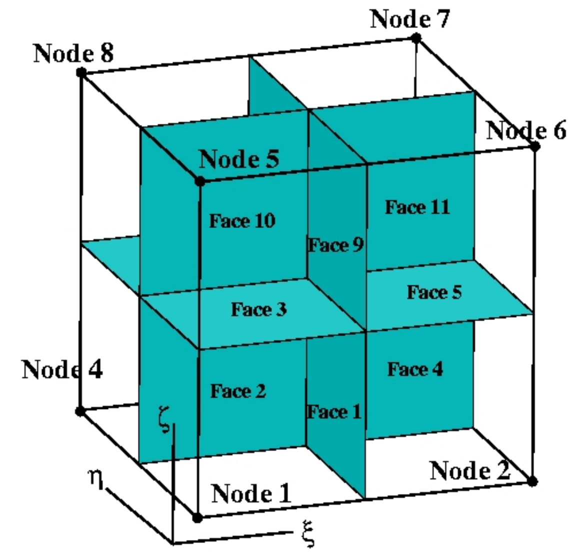
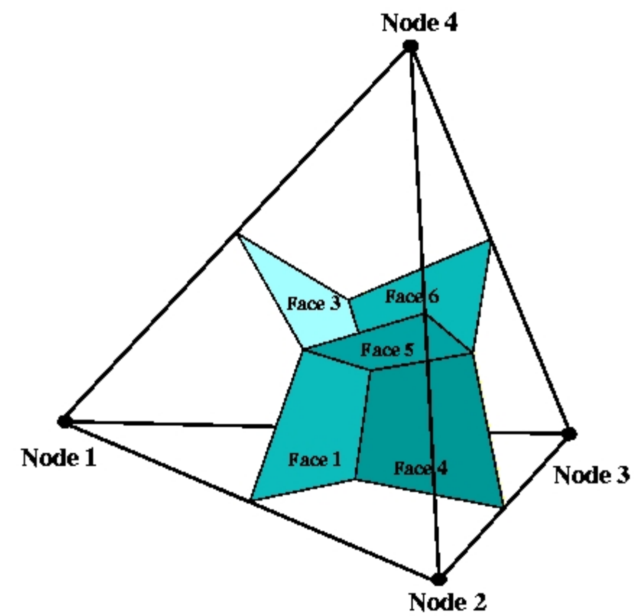


Fig. 1. CVFEM element and dual-volume definition for the low-order topologies.

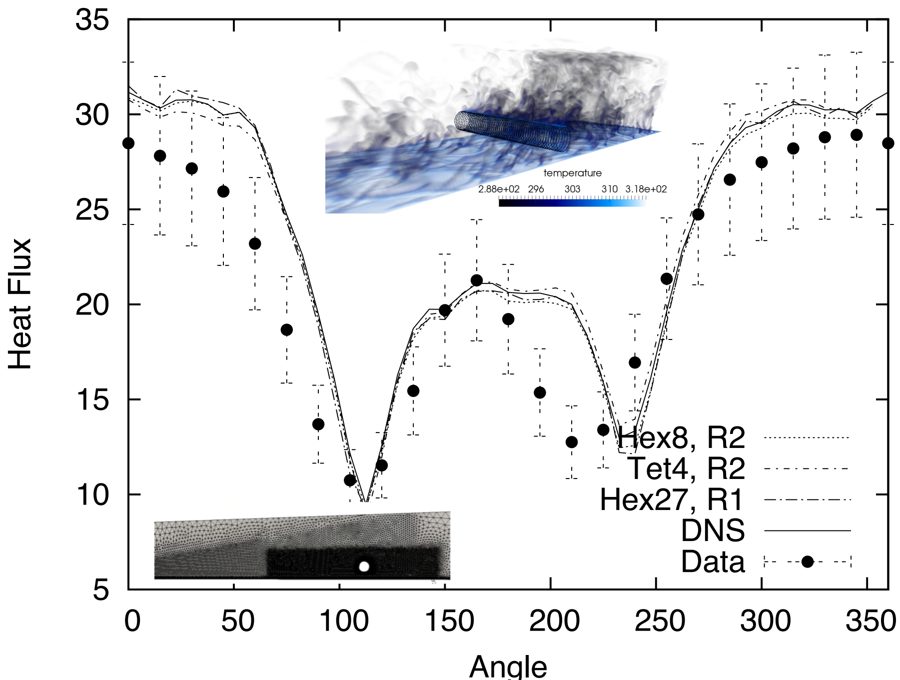


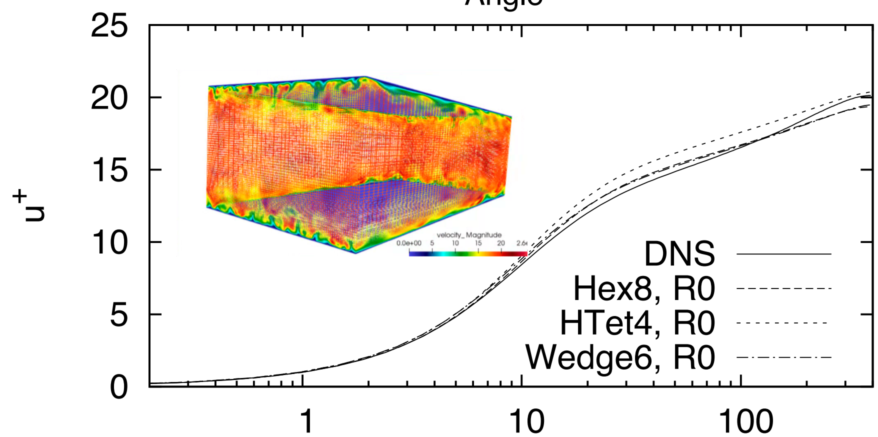


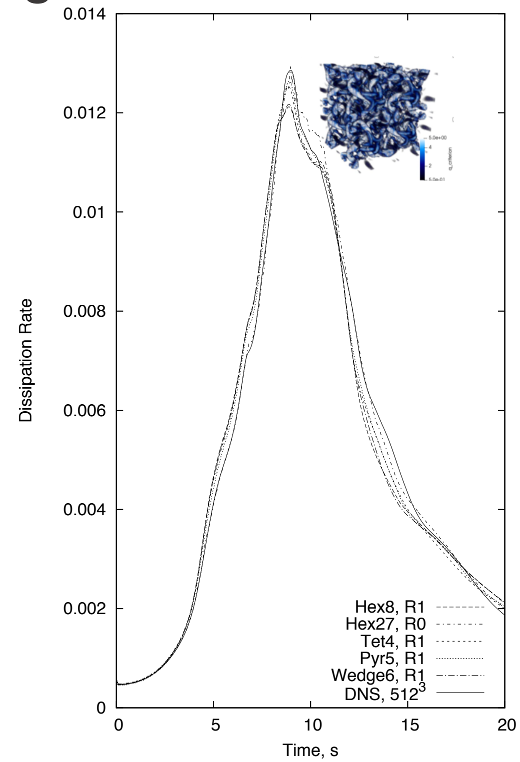
Domino, et. al, “An assessment of atypical mesh topologies for low-Mach large-eddy simulation” 2019

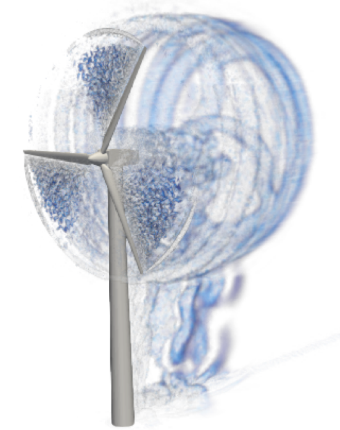
Recent Generalized Unstructured Findings

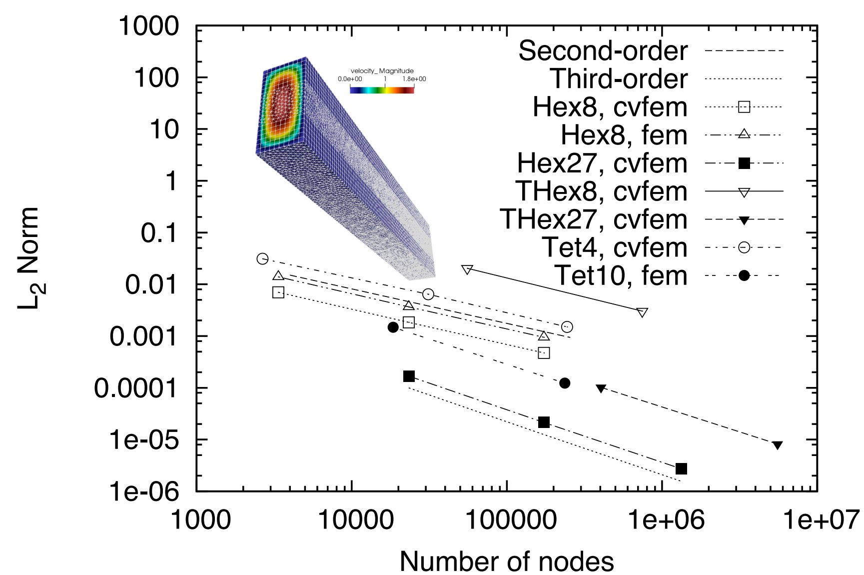
- Domino, et. al, "An assessment of atypical mesh topologies for low-Mach large-eddy simulation" 2019









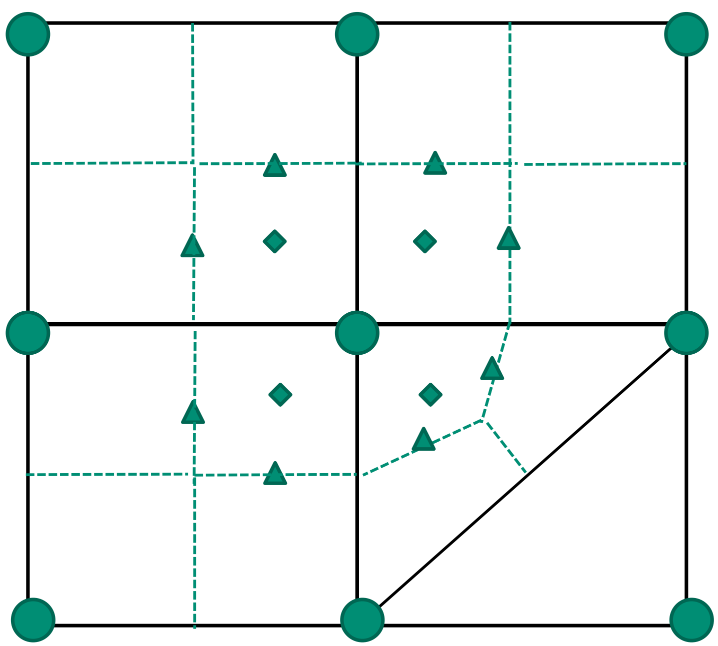


Equal Order Interpolation Edge-Based Vertex-Centered (EBVC) Finite Volume

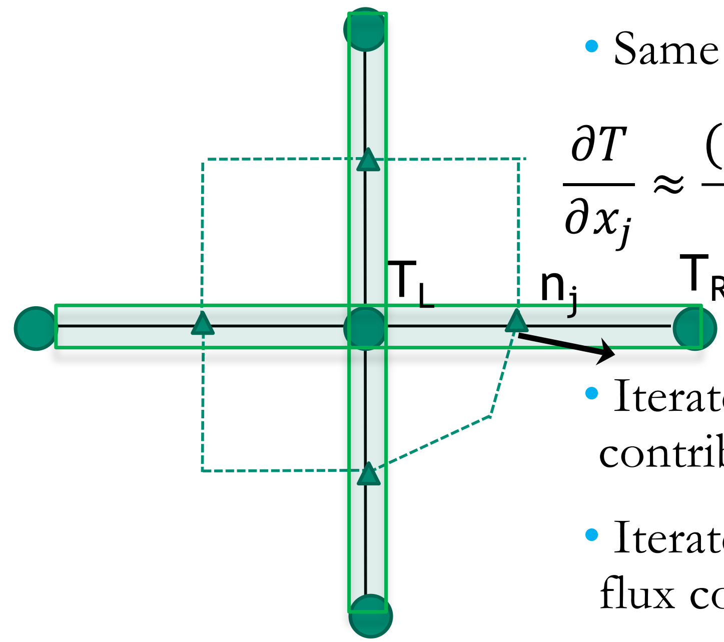
- All primitives are collocated at the vertices of the elements with equal-order interpolation
- A dual mesh is constructed to obtain flux and volume quadrature locations
- Classic two-state, "L" and "R" approach provides spatially second-order accuracy

▲ Surface quadrature point (area summed to edge)

◆ Volume quadrature point (sub-vol summed to node)



Dual-volume definition



Edge-based stencil

- Same grad-op as CC:

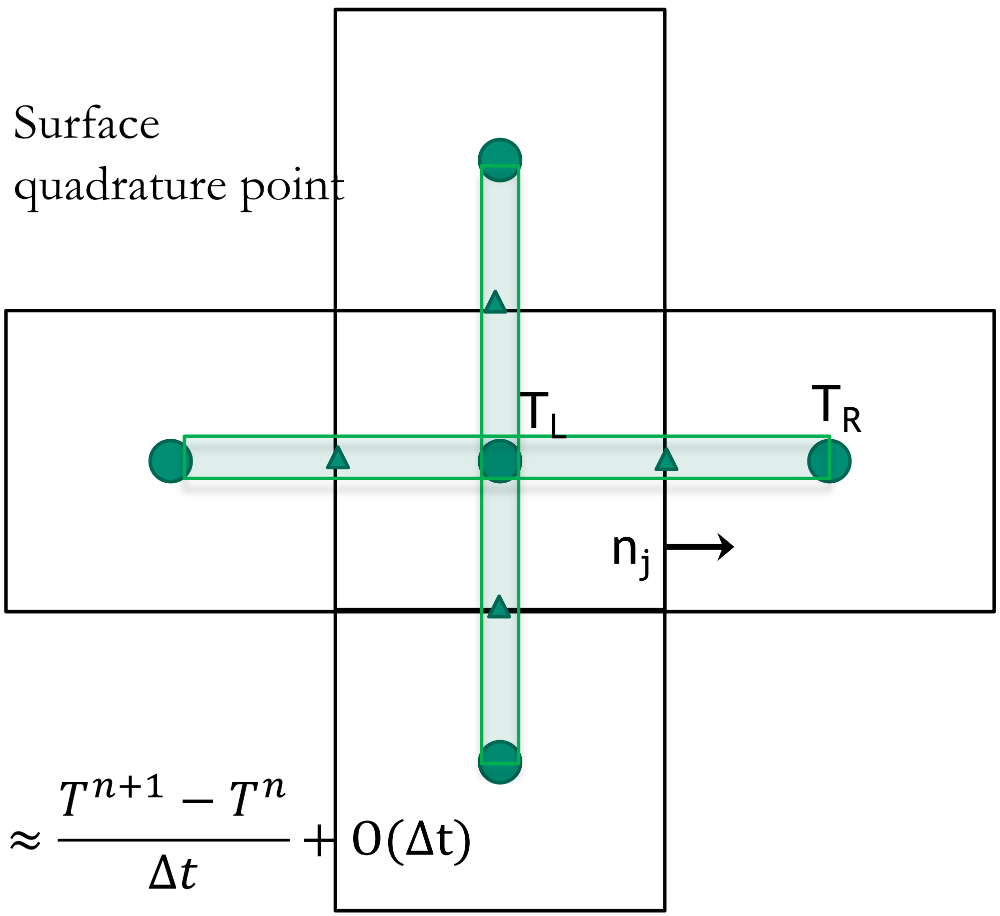
$$\frac{\partial T}{\partial x_j} \approx \frac{(T_R - T_L)n_j}{\|\Delta x_j\|} + O(\Delta x)$$

- Iterate nodes for volume contributions
- Iterate edges for surface flux contribution

Equal-Order Interpolation Cell-Centered (CC) Finite Volume

- All primitives are collocated at the cell-center of the element with equal-order interpolation
- Classic two-state, "L" and "R" approach provides spatially second-order accuracy

▲ Surface quadrature point



$$\frac{\partial T}{\partial t} \approx \frac{T^{n+1} - T^{n}}{\Delta t} + O(\Delta t)$$

- Consider a simple heat conduction model PDE,

$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} = 0$$

- Integrate over a control volume and use Gauss-Divergence,

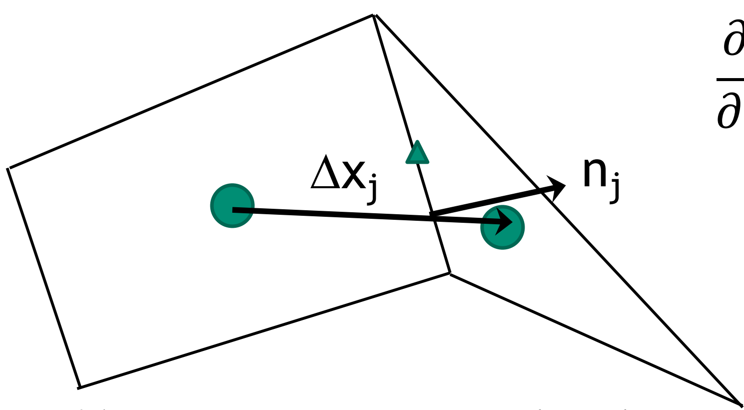
$$\int \rho C_p \frac{\partial T}{\partial t} dV \; - \int \lambda \frac{\partial T}{\partial x_j} n_j \, dS = 0$$

with: $\frac{\partial T}{\partial x_j} \approx \frac{(T_R - T_L) n_j}{\| \Delta x_j \|} + O(\Delta x)$

- Iterate element cell-centers for volume contributions (time/source)
- Iterate element faces for surface flux contribution

Typical Failings for Two-State Discretization Methods

- With two points, only a linear basis can be used.
- Therefore, unstructured CC and EBVC are limited to second-order spatial accuracy
- Non-orthogonality is problematic for gradient-operator



$$\frac{\partial T}{\partial x_j} = G_j T + \left[(T_R - T_L) - G_k T \Delta x_k\right] \frac{A_j}{A_l \Delta x_l}$$

With area vector defined by: $A_j = n_j dS$

- Above, $G_j T$ is a projected nodal gradient at the cell-center, or vertex center:
- Non-orthogonality is simply defined as the mis-alignment of the distance vector between the two "L" and "R" states and the surface normal

$$G_j T = \frac{\int T A_j}{\int dV}$$

- Both edge- and cell centered-based schemes show degraded accuracy on typical production meshes
- Several non-orthogonality approaches are available, for the best source, see Jasak
  - Jasak, "Error analysis and error estimation for the finite volume method with applications to fluid flow", Imperial College Dissertation, 1996

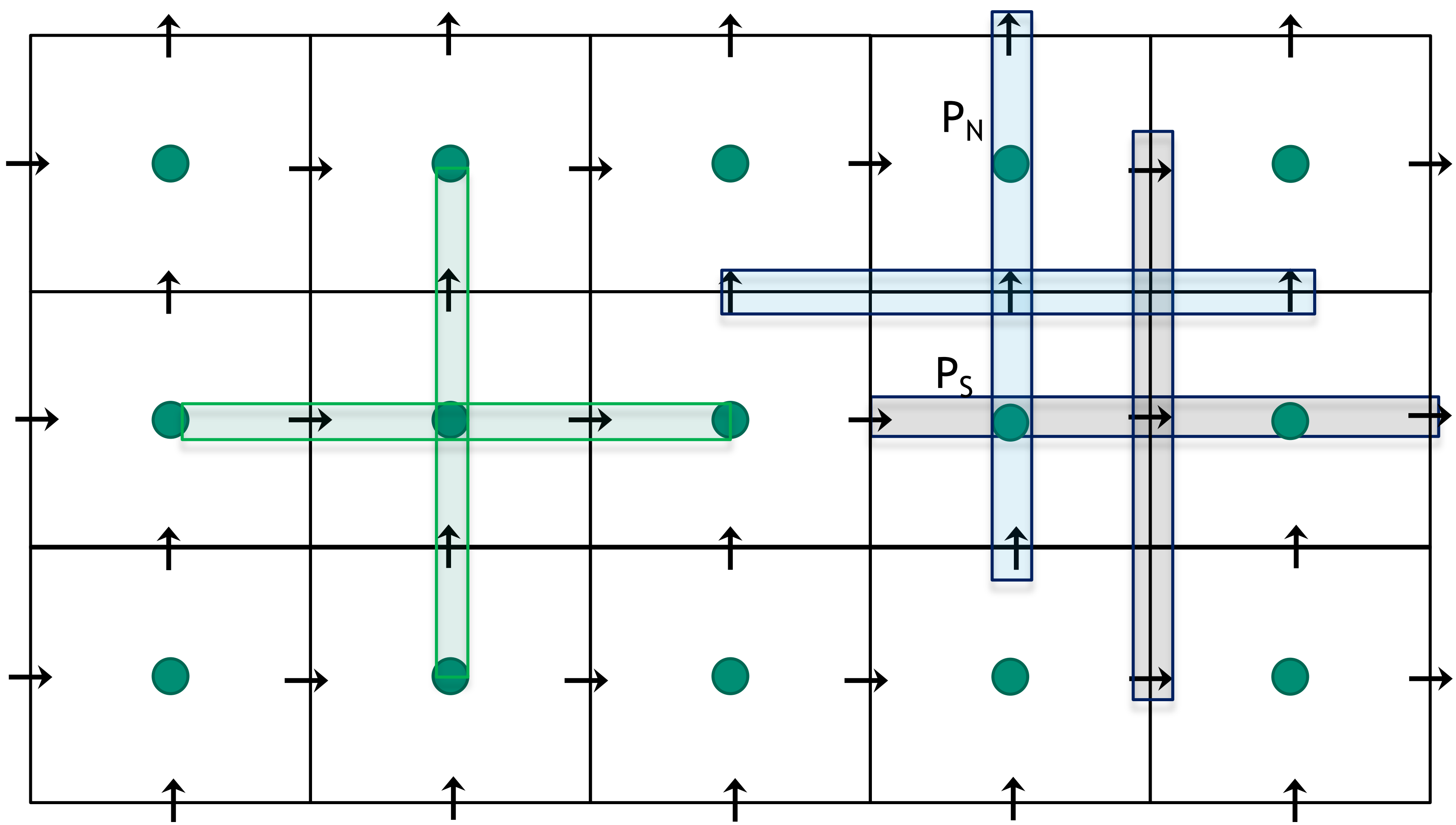
Classic Staggered Finite Volume

Stencil for CC-quantities

Stencil for x-velocity

Stencil for y-velocity

- Velocity degree-of-freedom is staggered relative to pressure and other primitives, e.g., enthalpy, mixture fraction, etc.



Attributes of a Staggered Scheme

- By design, non-orthogonality is absent, however, complex geometry will be stair-stepped
- From a fluids perspective, the operators are ideal, i.e., pressure gradient for momentum is compact, e.g., $(P_E - P_W)\Delta x^{-1}$
  - As will be seen in future lecture topics, the skew-adjoint nature of the Divergence operator, **D**, and Gradient operator, **G**, allows for a Laplace operator, **L** = **DG**
- Can be extended to higher-order
- Frequently, meshing complex geometries can be extremely difficult (consider our V27 example)

Common low-Mach Discretization Approaches: Conclusions

- Two-state methods, e.g., cell-centered and EBVC are attractive due to simplicity, however, suffer from non-orthogonality issues in the diffusion operator
- FEM provides a machinery to provide accurate discretizations on non-ideal meshes, however, the same diffusion operator suffers on high-aspect ratio meshes
- CVFEM is a hybrid method that contains the likeable attributes of both FV and FEM (same high-aspect ratio diffusion operator finding)
- Staggered arrangement is well suited for a class of fluid mechanics applications where low-order or simple geometries are found