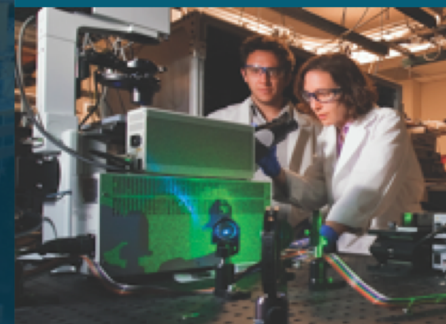
Guest Lecture Stanford ME469: Homework #1 Discussion



PRESENTED BY

Stefan P. Domino

Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND2018-4536 PE

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Homework #1 Discussion: Outline

- Discuss task 1: Nalu/reg_tests/test_files/dgNonConformalThreeBlade
- Discuss task 2: Nalu/reg_tests/test_files/fluidsPmrChtPeriodic
- Discuss task 3: specified pressure pipe flow

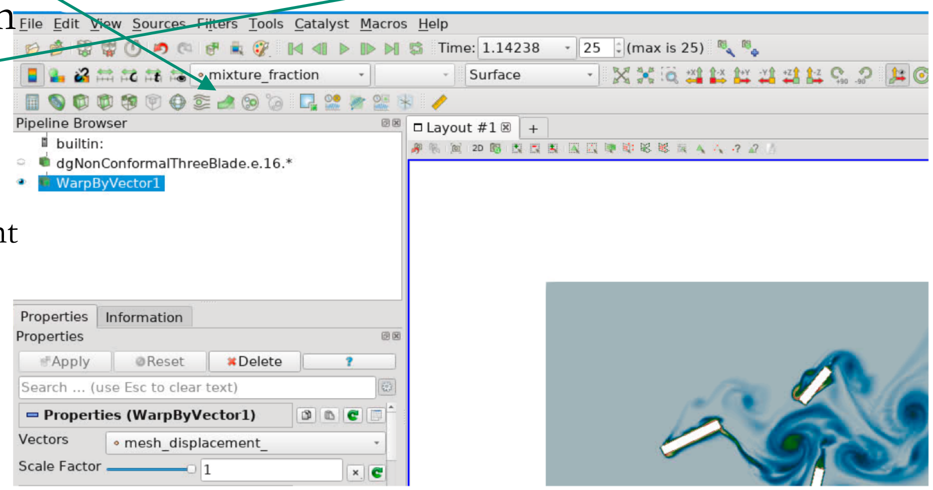
Wait… a significant departure from task 3

- Simple time/convection MMS for P=1
- Simple time/convection MMS for P=2
- Back to the pipe!
- Conclusions

Answer for Homework #1, Task 1 of 3

- Task 1: Run Nalu/reg_tests/test_files/dgNonConformalThreeBlade
  a. Modify the input file to increase termination_step_count to ~500:
  b. Visualize the flow field with displacements activated and provide a single image at the final step count.
  c. How does modification of the blade rotation (omega) affect the time step?
     i. time_stepping_type: adaptive
     ii. Courant# = $U^{RTM}\Delta t/\Delta x$ with $U^{RTM}=U-V^{mesh}$
     iii. As V^{mesh} increases, Δt decreases to meet a fixed Courant number specification of 2
  d. Report any modifications that resulted in catastrophic behavior, i.e., the simulation diverged. Document how you caused the simulation to diverge.
     i. Too large of a time step given rotation, omega
     ii. Initial time step too large
     iii. No open bc specified (rendering flow a low-speed compressible configuration)

```
Time_Integrators:
  - StandardTimeIntegrator:
      name: ti_1
      start_time: 0
      termination_step_count: 500
      time_stepping_type: adaptive
```




```
time_step_control:
    target_courant: 2.0
    time_step_change_factor: 1.15
```

Answer for Homework #1, Task 2 of 3

- Task 2: Run Nalu/reg_tests/test_files/fluidsPmrChtPeriodic
  a. Modify the input file to increase termination_step_count to ~500.
  b. Visualize the temperature, velocity, and radiative file (your choice) and provide a single image at the final step count.
  c. Modify the gravity constant such that the Rayleigh number 10x, 100x, etc. Report any findings; does the code benefit from a modification of initial time step size?
     i. Increased velocity magnitude from 0.16, 0.46, 1.5, and 3.7 m/s for gx1, gx10, gx100, gx1000
  d. What happens if you change the velocity hybrid parameter to: velocity: 0.0
     i. Far less advection stabilization is added. Former value of unity allows for velocity oscillations for cell Peclet number > 2
     ii. see: https://nalu.readthedocs.io/en/latest/source/theory/advectionStabilization.html

```
Time_Integrators:
  - StandardTimeIntegrator:
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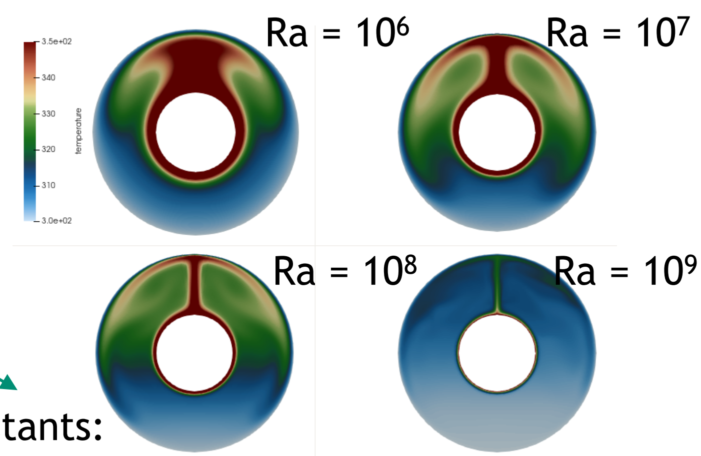
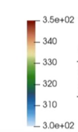


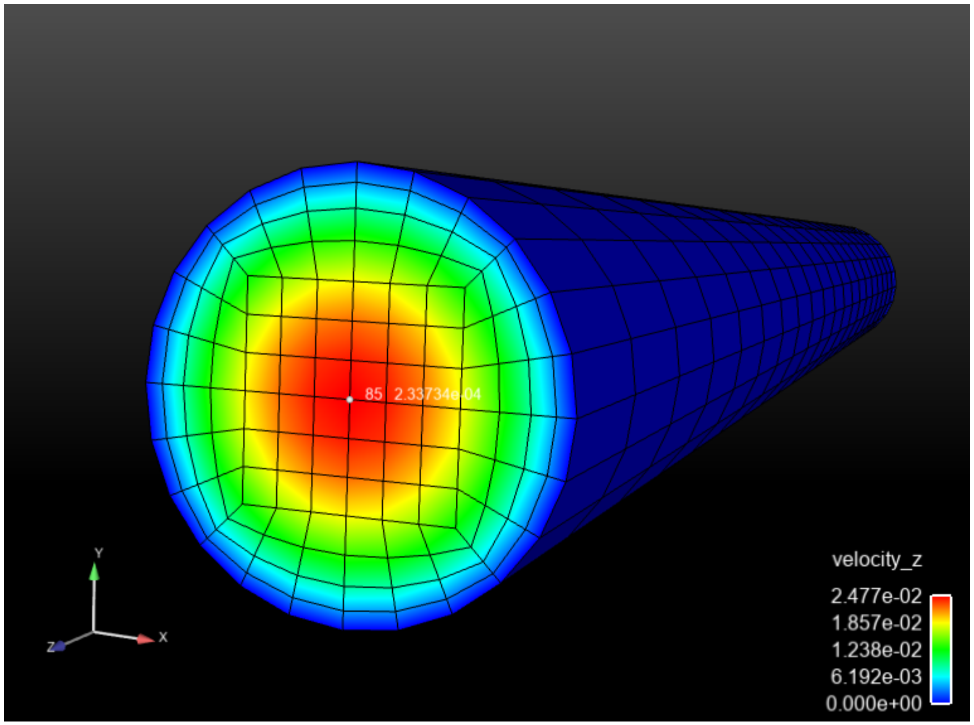

```
- user_constants:
  gravity: [0.0, -9810.0, 0.0]
```

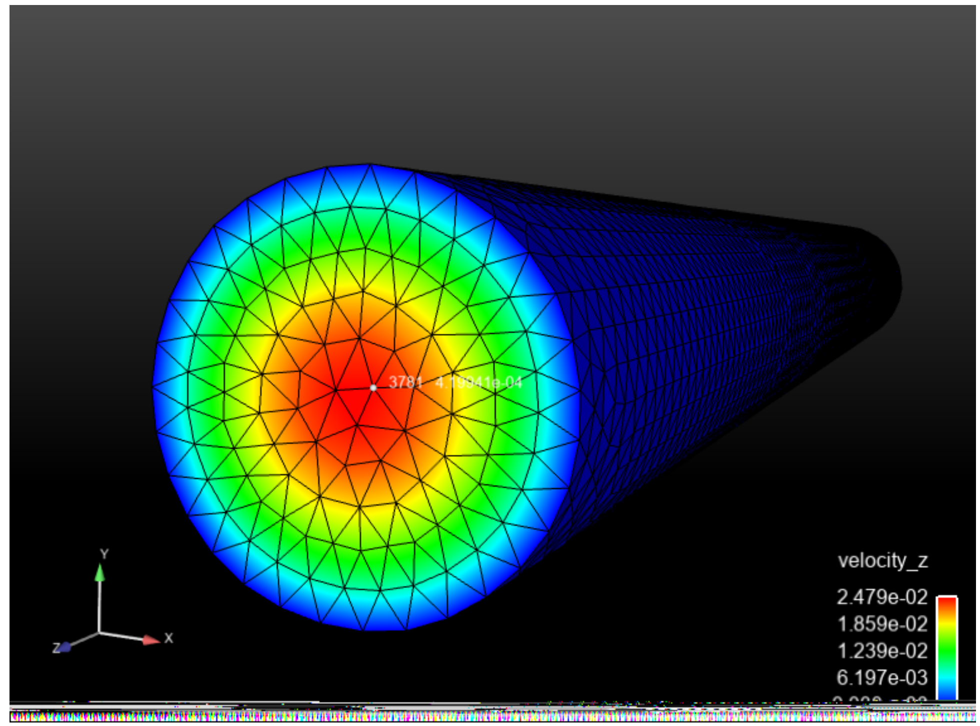
```
options:
  - hybrid_factor:
    velocity: 0.0
    enthalpy: 1.0
```



Ra ~ 10^9 velocity vector colored by temperature

Answer for Homework #1 Task 3: Specified Pressure Drop Laminar Pipe Flow:



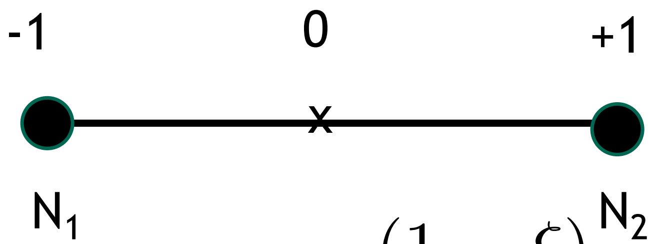


$$u(r) = u^{max}(1 - (\frac{r}{R})^2) \qquad u^{max} = \frac{\Delta p}{\Delta z}\frac{R^2}{4\mu}$$

First, let's think about this quadratic solution a bit more….

Element Integration: Physical Space

- Let us define a *linear* basis over a representative one-dimensional bar element with iso-parametric range of ξ: -1:+1



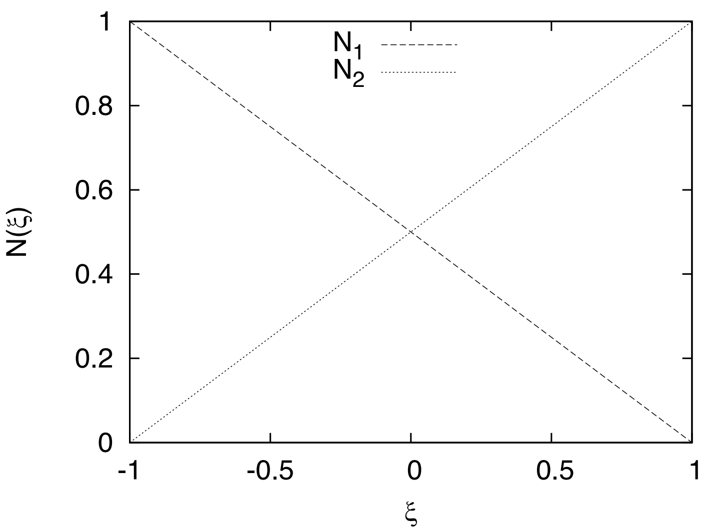
$$x(\xi) = \sum_n N_n x_n \qquad \frac{\partial x}{\partial \xi} = \sum_n \frac{\partial N_n}{\partial \xi} x_n$$

$$N_1(\xi) = \frac{(1-\xi)}{2}$$

$$N_2(\xi) = \frac{(1+\xi)}{2}$$

$$\frac{\partial N_1(\xi)}{\partial \xi} = -\frac{1}{2} \qquad \frac{\partial N_2(\xi)}{\partial \xi} = +\frac{1}{2}$$

$$\frac{\partial x}{\partial \xi} = -\frac{1}{2}x_1 + \frac{1}{2}x_2 = \frac{1}{2}(x_2 - x_1)$$



$$\frac{\partial N_n}{\partial x} = \frac{\frac{\partial N_n}{\partial \xi}}{\frac{1}{2}(x_2 - x_1)} \left\{ \begin{aligned} \frac{\partial N_1}{\partial x} &= \frac{-\frac{1}{2}}{\frac{1}{2}(x_2 - x_1)} = \frac{-1}{(x_2 - x_1)} \\ \frac{\partial N_2}{\partial x} &= \frac{\frac{1}{2}}{\frac{1}{2}(x_2 - x_1)} = \frac{+1}{(x_2 - x_1)} \end{aligned} \right.$$

$$\frac{\partial \phi_{ip}}{\partial x} = \frac{(\phi_2 - \phi_1)}{(x_2 - x_1)} \qquad \frac{\partial \phi_{ip}}{\partial x_j} = \sum_n \frac{\partial N_{ip,n}}{\partial x_j} \phi_n$$

Simple One-D MMS Example; General Form

- Consider a simple time/convection equation:

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} = 0 \qquad \text{with:} \qquad \phi^{mms}(x) = x^2$$

- One-D; let ρ and u_x be constant and unity: $\rho u_x \frac{\partial}{\partial x}\phi^{mms} = S^{mms} = 2x$

Gauss-Divergence

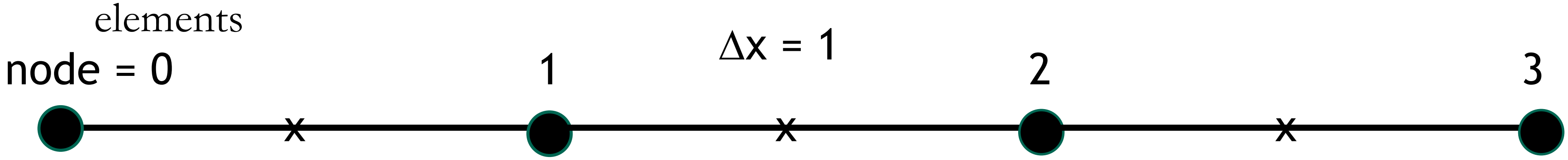
$$\int \frac{\partial}{\partial x_j}\rho\phi^{mms}u_j dV = \int S^{mms} dV \qquad \int \rho\phi^{mms}u_j n_j dS = \int S^{mms} dV$$

Discrete flux-based form: $\sum_{ip}^{scs} \rho_{ip}\phi_{ip}u_{ip,j}A_{ip,j} = \sum_{ip}^{scv} S_{ip}^{mms} Vol_{ip}$

With error: $\epsilon = \phi^{mms} - \phi$

Simple One-D MMS Example; Nodal Assemble of Source Term

- We will use a linear basis and solve this system over a small patch of linear bar elements



Boundary Conditions:
$\phi(x=0) = 0$
$\phi(x=3) = 9$

Recall general Eq:

$$\sum_{ip}^{scs} \rho_{ip}\phi_{ip}u_{ip,j}A_{ip,j} = \sum_{ip}^{scv} S_{ip}^{mms} Vol_{ip}$$

Simplified 1-D equation (unity density, x-velocity, and mesh spacing)

$$\sum_{ip}^{scs} \phi_{ip}A_{ip,x} = \sum_{ip}^{scv} S_{ip}^{mms} A_{ip,x}\Delta x \qquad \sum_{ip}^{scs} \phi_{ip} = \sum_{ip}^{scv} S_{ip}^{mms}$$

First, assign lhs and rhs to zero, iterate nodes to assemble right-hand side source term (2x):

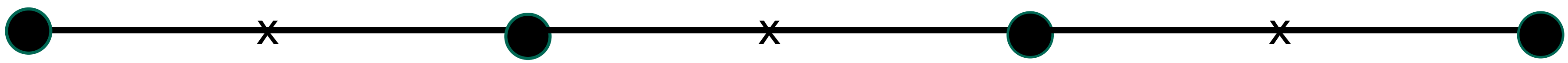
$$RHS = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 6 \end{pmatrix} \begin{matrix} \text{Node 0} \\ \text{Node 1} \\ \text{Node 2} \\ \text{Node 3} \end{matrix}$$

Simple One-D MMS Example; Edge-based assemble of convection

- We will use a linear basis and solve this system over a small patch of linear bar elements

$\Delta x = 1$

node = 0 1 2 3



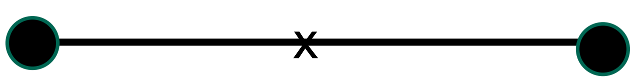
Recall, simplified equation with RHS from source term already provided

$$\sum_{ip}^{scs} \phi_{ip} = \sum_{ip}^{scv} S_{ip}^{mms} \qquad RHS = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 6 \end{pmatrix}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

0 1



$$\phi_{ip} = \frac{(\phi_1 + \phi_0)}{2}$$

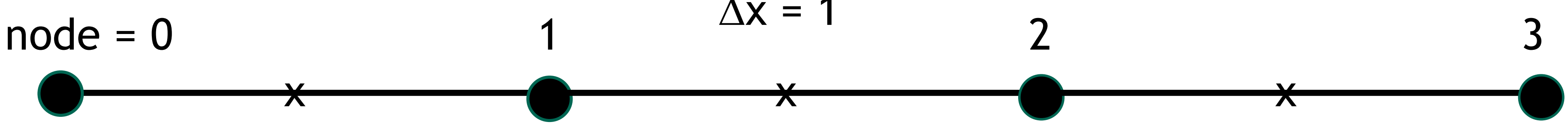
Edge 1

$$lhs_0 \mathrel{+}= \frac{(\phi_1 + \phi_0)}{2}$$

$$lhs_1 \mathrel{-}= \frac{(\phi_1 + \phi_0)}{2}$$

Simple One-D MMS Example; Edge-based assemble of convection

- We will use a linear basis and solve this system over a small patch of linear bar elements



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Iterate elements with a simple left-hand side rule: += L and -=R
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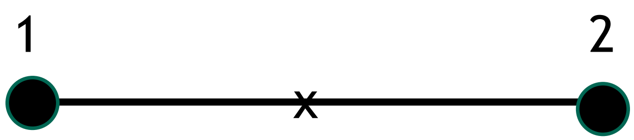


$$\phi_{ip} = \frac{(\phi_2 + \phi_1)}{2}$$

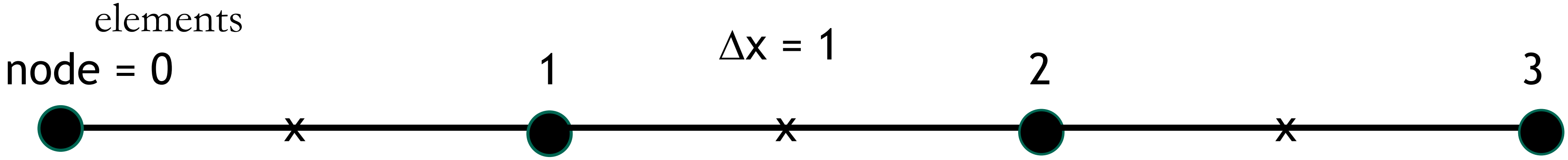
$$lhs_1 \mathrel{+}= \frac{(\phi_2 + \phi_1)}{2}$$

$$lhs_2 \mathrel{-}= \frac{(\phi_2 + \phi_1)}{2}$$

Edge 2

Simple One-D MMS Example; Linear CVFEM Assembly

- We will use a linear basis and solve this system over a small patch of linear bar elements



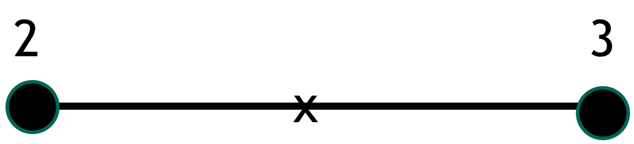
Recall, simplified equation with RHS from source term already provided

$$\sum_{ip}^{scs} \phi_{ip} = \sum_{ip}^{scv} S_{ip}^{mms}$$

$$RHS = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 6 \end{pmatrix}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)



$$\phi_{ip} = \frac{(\phi_3 + \phi_2)}{2}$$

$$lhs_2 \mathrel{+}= \frac{(\phi_3 + \phi_2)}{2}$$

$$lhs_3 \mathrel{-}= \frac{(\phi_3 + \phi_2)}{2}$$

Edge 3

Simple One-D MMS Example; Collect all of the lhs entries

$$lhs_0 \mathrel{+}= \frac{(\phi_1 + \phi_0)}{2}$$

$$lhs_1 \mathrel{-}= \frac{(\phi_1 + \phi_0)}{2}$$

$$lhs_1 \mathrel{+}= \frac{(\phi_2 + \phi_1)}{2}$$

$$lhs_2 \mathrel{-}= \frac{(\phi_2 + \phi_1)}{2}$$

$$lhs_2 \mathrel{+}= \frac{(\phi_3 + \phi_2)}{2}$$

$$lhs_3 \mathrel{-}= \frac{(\phi_3 + \phi_2)}{2}$$

$$A = \begin{pmatrix} +\frac{1}{2} & +\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

$$\begin{pmatrix} +\frac{1}{2} & +\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 6 \end{pmatrix}$$

Correct for BCs:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 9 \end{pmatrix}$$

Solution is exact!

$$\begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 4 \\ 9 \end{pmatrix}$$

Simple One-D MMS Example; General Form (new source)

- Consider a simple time/convection equation:

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} = 0 \qquad \text{with:} \qquad \phi^{mms}(x) = \cancel{x^2}\ x^3$$

- One-D; let ρ and u_x be constant and unity: $\rho u_x \frac{\partial}{\partial x}\phi^{mms} = S^{mms} = \cancel{2x}\ 3x^2$

Gauss-Divergence

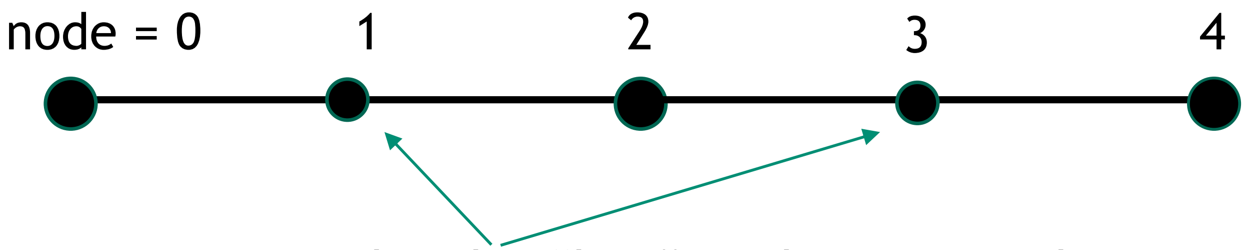
$$\int \frac{\partial}{\partial x_j}\rho\phi^{mms}u_j dV = \int S^{mms} dV \qquad \int \rho\phi^{mms}u_j n_j dS = \int S^{mms} dV$$

Discrete flux-based form: $\sum_{ip}^{scs} \rho_{ip}\phi_{ip}u_{ip,j}A_{ip,j} = \sum_{ip}^{scv} S_{ip}^{mms} Vol_{ip}$

With error: $\epsilon = \phi^{mms} - \phi$

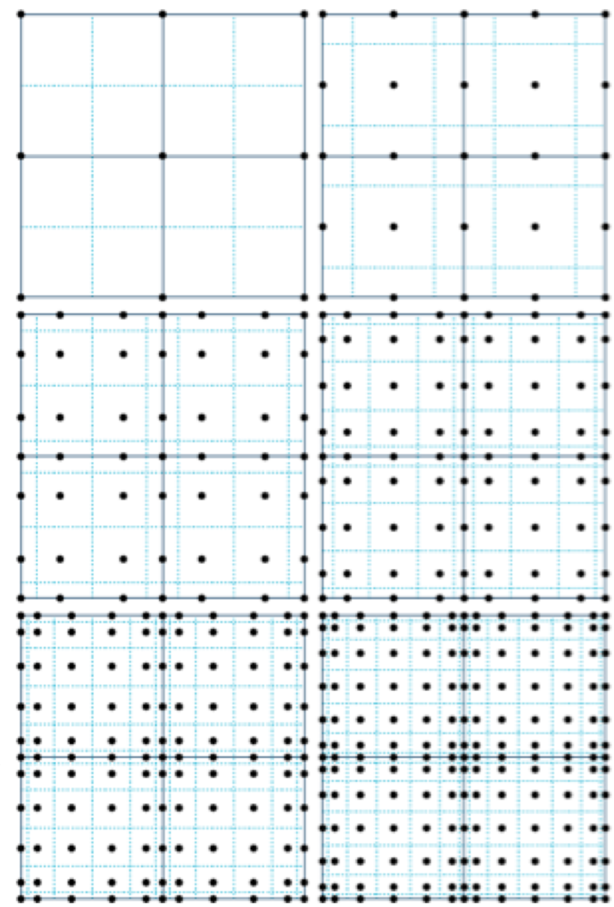
Simple One-D MMS Example; Quadratic CVFEM Assembly

- We will use a quadratic basis and solve this system over a small patch of quadratic bar elements



- New promoted nodes "live" at the Gauss-Lobatto points while dual volume lives at the Gauss-Lagendre points: +/- sqrt(3)/3
- Number of quadrature points for accurate integration scales as:
    - 2*numPts – 1 = polynomial order
    - "2x2" quadrature will sufficiently integrate a quadratic basis
    - Using single point quadrature would provide results that simply replicate uniform refinement of the low-order mesh.

Replicating the previous example with the new basis would again demonstrate exact prediction of nodal results!



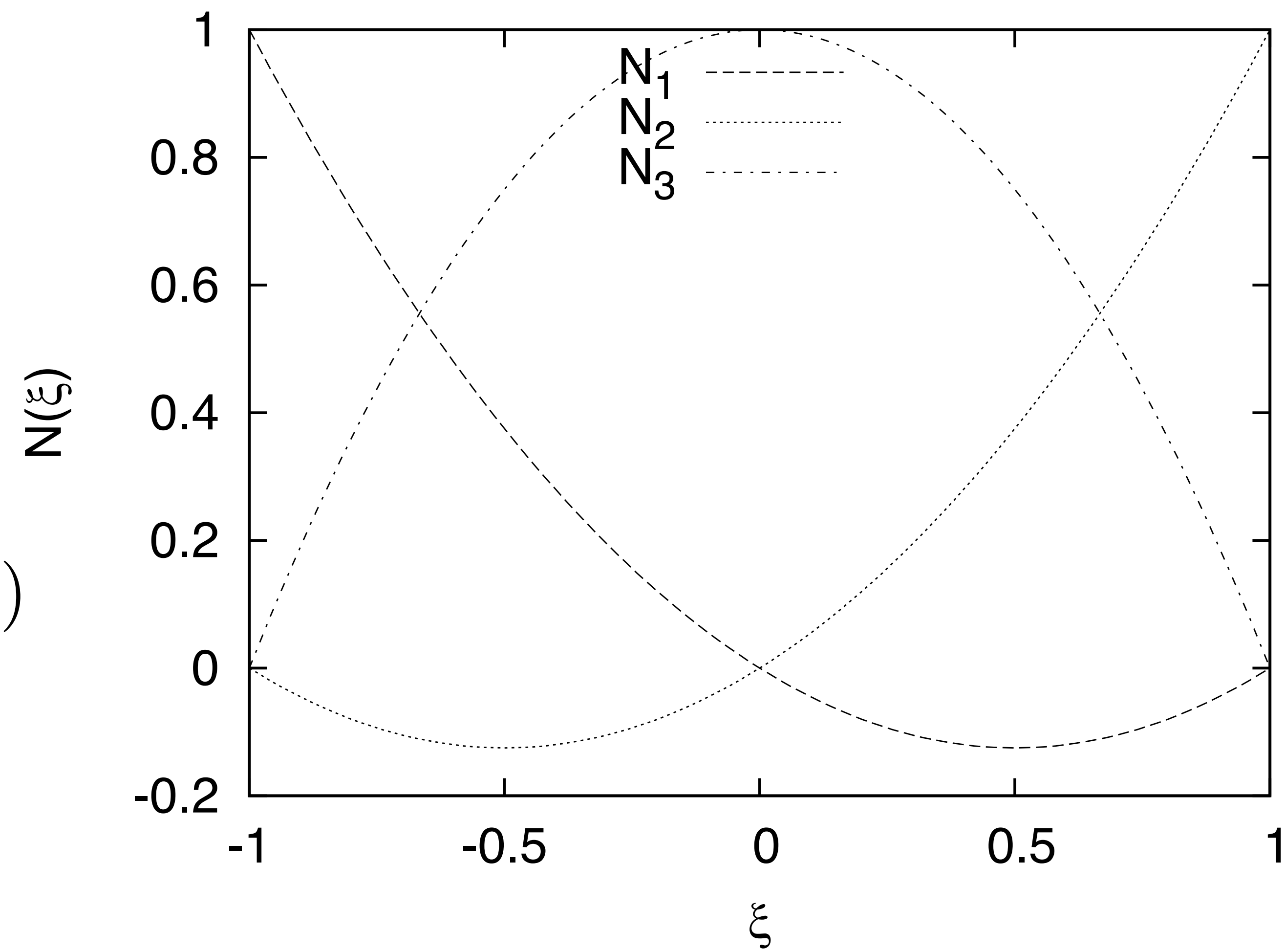
O(P) basis: $O(\Delta x)^{P+1}$ accuracy

Example of a Quadratic Basis Function

$$N_1 = \frac{-\xi(1-\xi)}{2}$$

$$N_2 = \frac{\xi(1+\xi)}{2}$$

$$N_2 = (1-\xi)(1+\xi)$$



Answer for Homework #1 Task 3: Specified Pressure Drop Laminar Pipe Flow:

- Location: https://github.com/spdomin/Present/tree/master/stanfordMe469/hw/one
- You will modify the input file to provide the density, viscosity and pressure drop to achieve $Re^{\tau} = 10$ and report on the differences between the simulation and analytical centerline velocity.
- Specifications:
  - $Re^{\tau} = 10$
  - Pipe diameter, D = 0.01 m
  - Pipe Length, L = 0.1 m

i. Perform a global momentum balance to determine the pressure gradient. dp/dz as a function of the wall shear stress , τ_w.
   i. Momentum Balance: $dp/dz = 4 \tau_w / D$

ii. Given $Re^{\tau} = \rho u^{\tau} D / \mu$ and $\tau_w = \rho (u^{\tau})^2$, where u^{τ} is the wall friction velocity, report the required pressure gradient required for the desired $Re^{\tau} = 10$.
   i. $\Delta p/\Delta z = 40.0\text{e-}3$ Pa/m with $\Delta Z = 0.1$ m

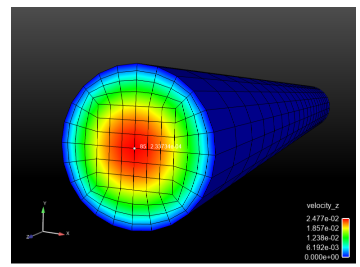
iii. Modify the input file to specify the proper density, viscosity and open pressure specification (look for the pressure specification under open_user_data).
   i. $\rho = 1.0$ kg/m^3 $\mu = 1.0\text{e-}5$

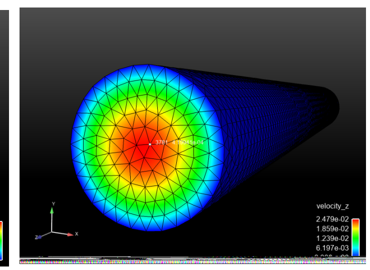
iv. Run both the Hex8 and Tet4 input file and compare the simulation centerline velocity to the analytical result (feel free to derive or simply report the functional form).
   i. Analytical centerline is 2.5e-2 m/s
   ii. Close, however, not exact for this second-order functional form due to geometry errors.
   iii. Anyone try a 1x1x10 developing square pipe?

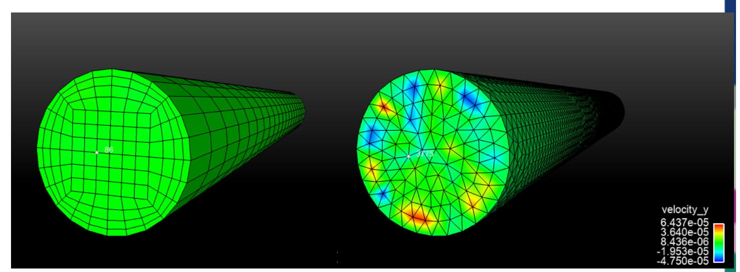
v. Capture any findings between the Hex8 and Tet4 simulation, e.g., simulation time, velocity component qualitative differences, convergence, etc.

```
- open_boundary_condition: bc_left
    target_name: surface_2
    open_user_data:
      pressure: 40.0e-4
      velocity: [0.0,0.0,0.0]

- open_boundary_condition: bc_right
    target_name: surface_1
    open_user_data:
      pressure: 0.0
      velocity: [0.0,0.0,0.0]
```







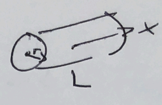
Hex wall-normal velocity is O(1e-15) while Tet is O(1e-6) m/s

$$u(R) = u^{Max} [1-(r/R)^2]$$
$$u^{Max} = \Delta p/\Delta z \; R^2 / (4 \mu)$$

Pipe Flow Derivation

Pipe-flow; 3-D specified pressure drop. (1)

$$\int \frac{\partial P}{\partial x}\, dV = \int \tau_w \, dA$$



$$\frac{\partial P}{\partial x} \cdot \cancel{\pi} r^{\cancel{2}} \cdot \cancel{L} = \tau_w \cdot 2 \cancel{\pi} \cancel{r} \cdot \cancel{L}$$

$$\boxed{\frac{\partial P}{\partial x} = \frac{\tau_w 2}{r}} \; ; \; 2r = D \quad r = D/2.$$

$$= \frac{4 \tau_w}{D}$$

$$\tau_w = -\mu \frac{\partial u}{\partial r}$$

$$\frac{dP}{dx}\frac{r}{2} = -\mu \frac{\partial u}{\partial r} \qquad \frac{\partial u}{\partial r} = -\frac{r}{2\mu}\frac{\partial P}{\partial x}.$$

$$u(r) = -\frac{r^2}{4\mu}\frac{\partial P}{\partial x} + C$$

@ $r = R$; $u = 0$

$$u(r=R) = 0 = -\frac{R^2}{4\mu}\frac{\partial P}{\partial x} + C$$

$$C = \frac{R^2}{4\mu}\frac{\partial P}{\partial x}$$

$$u(r) = -\frac{r^2}{4\mu}\frac{\partial P}{\partial x} + \frac{R^2}{4\mu}\frac{\partial P}{\partial x}$$

$$= \frac{1}{4\mu}\frac{\partial P}{\partial x}\left(R^2 - r^2\right) = \frac{R^2}{4\mu}\frac{\partial P}{\partial x}\left(1 - \frac{r^2}{R^2}\right)$$

$$\boxed{u^{max} = \frac{R^2}{4\mu}\frac{\partial P}{\partial x}}$$

Review: $u(r) = \frac{R^2}{4\mu}\frac{\partial P}{\partial z}\left(1 - \frac{r^2}{R^2}\right)$ (2)

$$u^{max} = \frac{R^2}{4\mu}\frac{\partial P}{\partial z} = \frac{R^2}{4\mu}\frac{\Delta P}{\Delta z} = \frac{D^2}{16\mu}\frac{\Delta P}{\Delta z}$$

$$Re^\tau = \frac{\rho u^\tau D}{\mu} \equiv 10 \qquad D = 0.01\,m \quad \Delta z = 0.1\,m$$

$$\tau_w = \rho u^{\tau 2} \qquad u^\tau = \frac{Re^\tau \mu}{\rho D}$$

$$\tau_w = \rho \left(\frac{Re^\tau \mu}{\rho D}\right)^2$$

$$\frac{\Delta P}{\Delta z} = \frac{4 \tau_w}{D} = \frac{4 \rho}{D}\left(\frac{Re^\tau \mu}{\rho D}\right)^2.$$

Let $\rho = 1.0 \frac{kg}{m^3}$ $\quad \mu = 1.0E{-5} \frac{kg}{m \cdot s}$.

$$\frac{\Delta P}{\Delta z} = \frac{4(1)}{0.01}\left(\frac{10 \cdot (1E{-5})}{(1)\, 0.01}\right)^2 = 40.0E{-3}$$

$$\Delta P = (40.0E{-3})(0.1) = 4.0E{-3}$$

$$u^{max} = \frac{(0.01/2)^2}{(4)(E{-5})} \cdot 40.0E{-3} = 2.5E{-2}\,\frac{m}{s}$$

Convince Yourself!
Removal of Geometric Error Induced by the Pipe

Domino et al., "Verification for Multi-Mechanics Applications ", AIAA, 2007

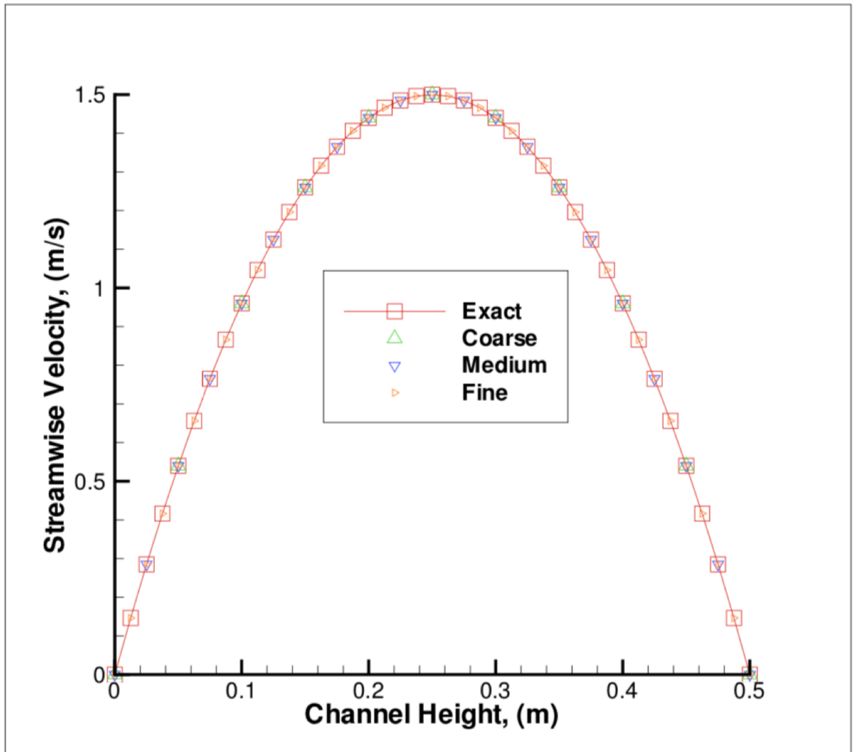


Figure 1. Comparision between analytical and computational solution on three meshes using the MUSCL operator.

$$-\frac{1}{\mu}\frac{\partial p}{\partial x} = \frac{\partial^2 u}{\partial y^2}$$

BCs:

$$u(y=0) = 0$$
$$u(y=H) = 0$$

$$u(y) = -\frac{1}{2\mu}\frac{\partial p}{\partial x}\left(yH - y^2\right)$$

Note: A common norm methodology to alleviate this slight confusion is to integrate over the domain using a consistent mass matrix:

$$L_1 = \int w(\phi - \phi^{mms})dV$$

For P=1, this procedure interpolates the quadratic solution using the underlying basis and reverts to displaying a clear second-order error for ε vs Δx

Homework #1 Discussion: Conclusions

- A P-order underlying polynomial basis will provide a P+1 integrated error
- Geometric fidelity for complex geometries is required for accurate solutions