Vascular Fluid Structure Simulation

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Overview

- Utilize a set of programs to simulate the blood flow in arteries
- Evaluates the stability of implemented solvers to handle fluid structure interaction problems
- Use continuous Galerkin finite element method and will extend to discontinuous Galerkin finite element method
- Utilize DIEL to solve weak coupling equations

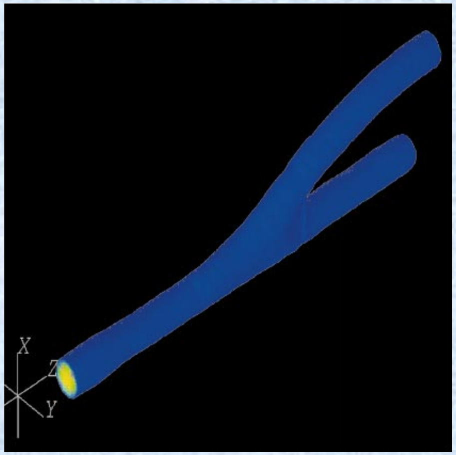
Fluid-Structure Interactions

- Blood flow causes deformation of the vessel wall and deformation of the wall changes the boundary conditions of blood flow.
- Two components
  - Fluid (blood) modeled by Navier-Stokes equations
  - Solid structure (vessel wall) modeled by partial differential equations of 1D, 2D and 3D, giving radial and longitudinal deformation of wall from its resting state
- Develop a coupling strategy to solve fluid-structure equations

Fluid Structure Interaction Equations

Fluid Equations(INS)

$$\begin{cases} \boldsymbol{u}_t - \dfrac{1}{\mathrm{Re}} \nabla^2 \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \boldsymbol{0} \\ \nabla \cdot \boldsymbol{u} = 0 \end{cases}$$



Boundary Interactions

$$[u]_{r=a} = \frac{\partial \eta}{\partial t} \quad \text{and} \quad [w]_{r=a} = \frac{\partial \xi}{\partial t}$$

Structure Equations

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{\tau}^s - \boldsymbol{\nabla} p^s &= \boldsymbol{0}, \\ \det(\boldsymbol{F}) &= 1, \end{aligned}$$

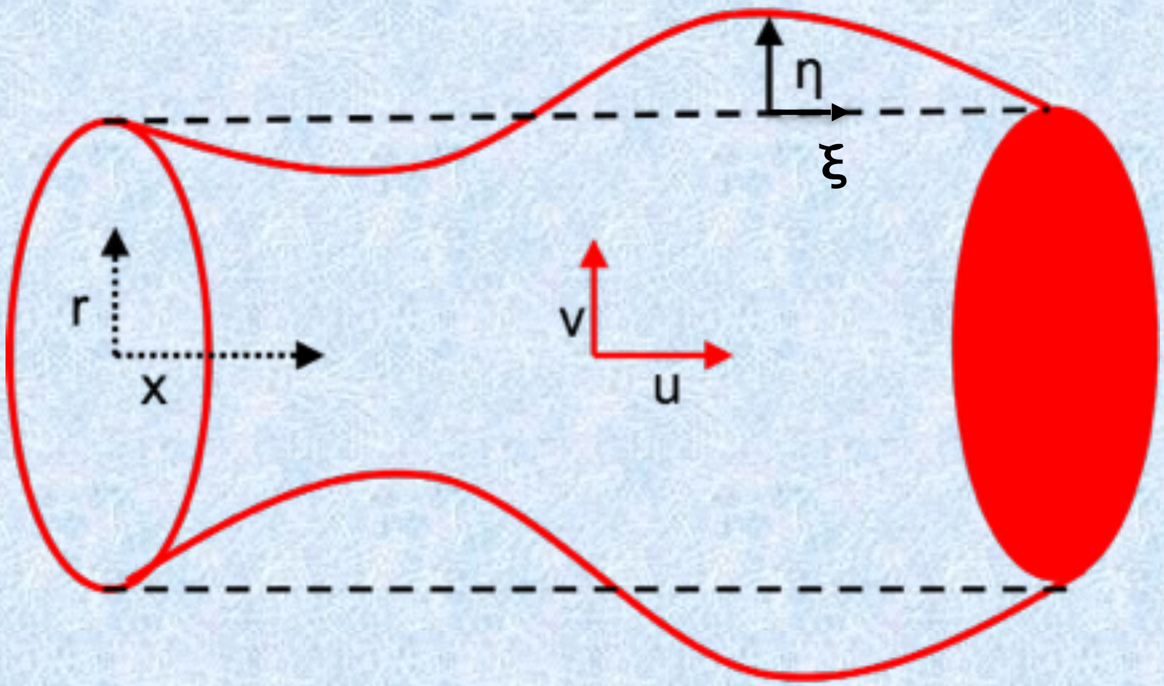
$$\boldsymbol{\tau}^s = G\left(\boldsymbol{F} \cdot \boldsymbol{F}^T - \boldsymbol{I}\right),$$

$$\boldsymbol{F} = (\vec{\nabla}_0 \vec{x})^{\mathrm{T}},$$

Algorithm

1. Solve Navier-Stokes equations(INS) for blood flow velocity and pressure
2. Solve structure equations for radial and longitudinal deformations of the vessel wall
3. Update the mesh
4. Update radial velocity at vessel wall
5. t = t + Δt
6. Continue from Step 1

1D structure and 2D axisymmetric Artery model



Quarteroni, Alfio; Tuveri, Massimiliano; Veneziani, Alessandro. “Computational vascular fluid dynamics: problems, models, and methods" Comput Visual Sci 2:163-197 (2000).

Axisymmetric Navier-Stokes equations

- Blood flow is axisymmetric flow with the assumption of no tangential velocity
- Can use cylindrical representation of the incompressible Navier–Stokes equations with no tangential velocity:

$$
\begin{aligned}
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + w\frac{\partial u}{\partial x} &= -\frac{1}{\rho}\frac{\partial p}{\partial r} + \nu\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial x^2} - \frac{u}{r^2}\right) \\
\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial x} &= -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial x^2}\right) \\
\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{\partial w}{\partial x} &= 0,
\end{aligned}
$$

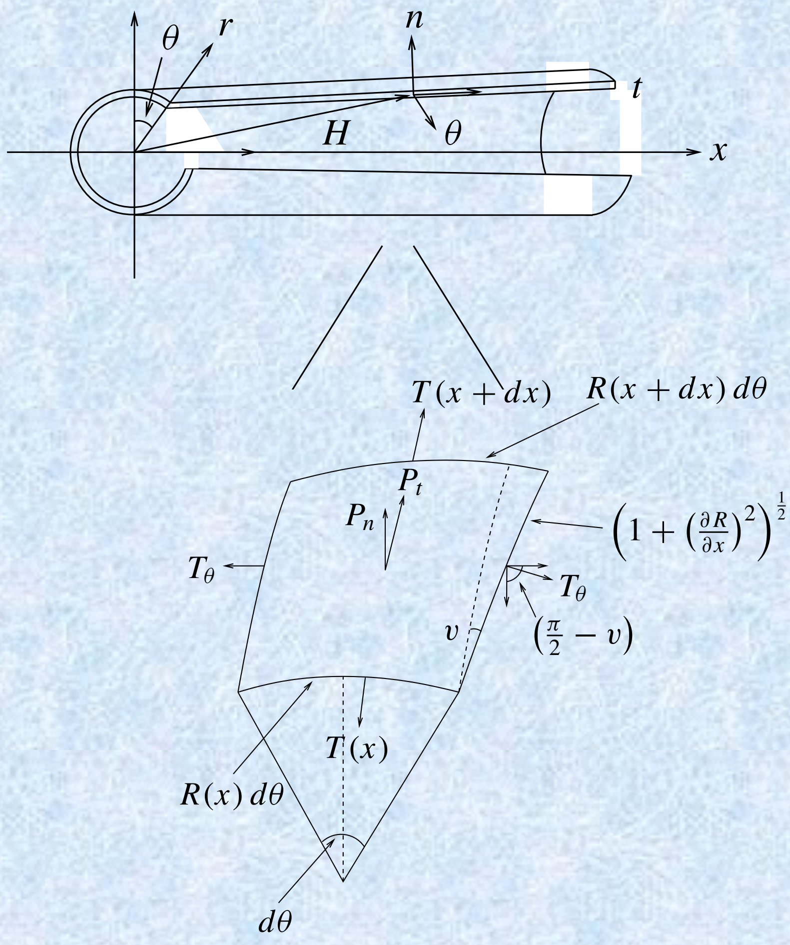
1D structure formulation

- 1D structure equations are based on the Ottesen's formula.
- The structure equations come from the forces acting on the wall
- He first balances internal(T) and external forces(P).
- Then reformulates P into T:

$$P_n = \kappa_\theta T_\theta + \kappa_t T_t,$$

where κ_i, $i = \theta, t$, is the curvature in the i direction.

- Thus, get the 1D structure equations



1D Structure Equations

Vessel Wall Equations

$$M_0 \frac{\partial^2 \xi}{\partial t^2} + L_x \frac{\partial \xi}{\partial t} + K_x \xi$$

$$= \frac{E_x h}{1-\sigma_\theta \sigma_x} \frac{\partial^2 \xi}{\partial x^2} + \left(\frac{T_{t_0} - T_{\theta_0}}{a} - \frac{E_x h \sigma_x}{a(1-\sigma_\theta \sigma_x)}\right) \frac{\partial \eta}{\partial x} - \mu\left[\frac{\partial w}{\partial r} + \frac{\partial u}{\partial x}\right]_a$$

$$M_0 \frac{\partial^2 \eta}{\partial t^2} + L_r \frac{\partial \eta}{\partial t} + K_r \eta$$

$$= T_{t_0} \frac{\partial^2 \eta}{\partial x^2} + \left(\frac{T_{\theta_0}}{a^2} - \frac{E_\theta h}{a^2(1-\sigma_\theta \sigma_x)}\right)\eta + \frac{E_\theta h \sigma_\theta}{a(1-\sigma_\theta \sigma_x)} \frac{\partial \xi}{\partial x} + \left[p - 2\mu \frac{\partial u}{\partial r}\right]_a$$

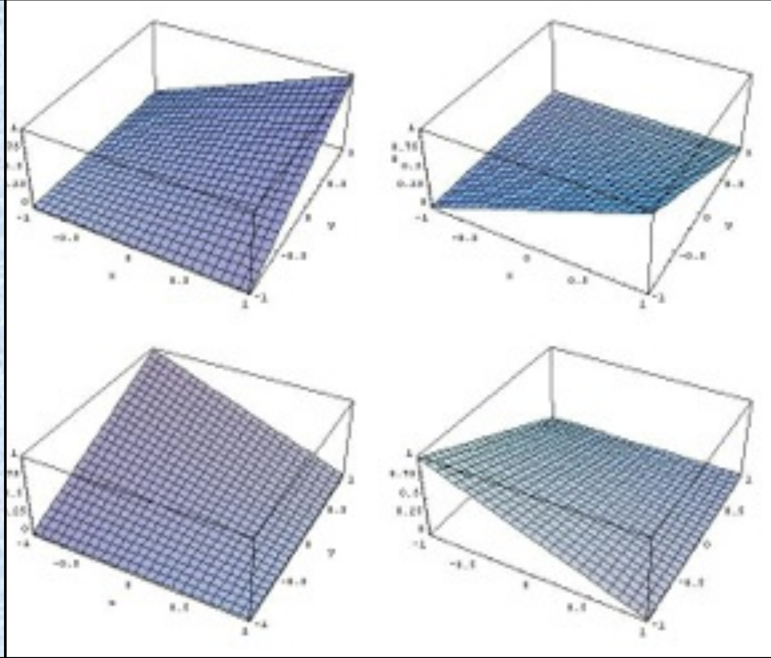
where E_i, $i = \theta, t$, is Young's modulus in the ith direction; h is the wall thickness; σ_i, $i = \theta, x$, is the Poisson ratio in the ith direction; and ϵ_i, $i = \theta, x$, is the displacement relative to the reference state;

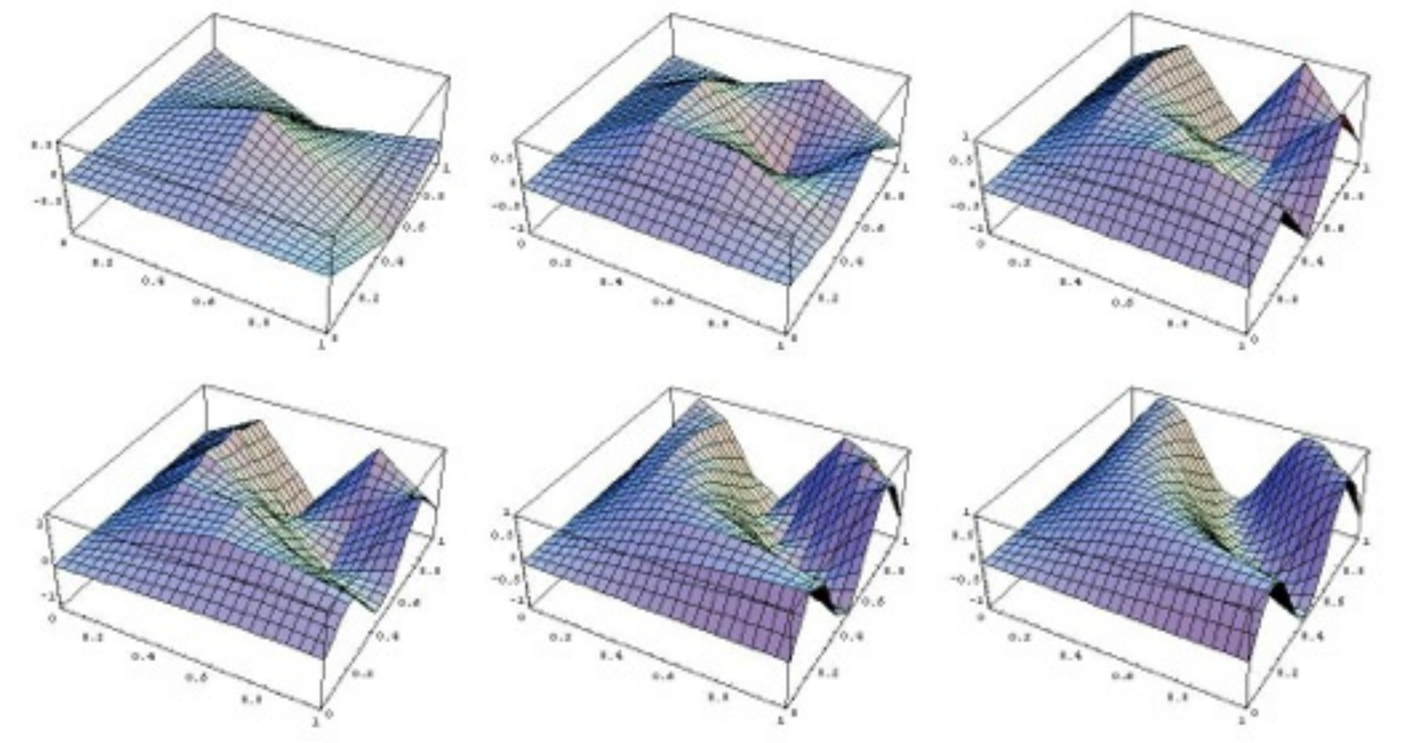
Algorithm for 2D axisymmetric Artery

1. Solve Navier-Stokes equations(INS) for blood flow velocity(u,w) and pressure(p) on a 2D mesh
2. Solve structure equations for radial and longitudinal deformations(η,ξ) of the vessel wall on a 1D mesh
3. Update the mesh using η , ξ , since vessel wall has moved
4. Update radial velocity at vessel wall, since radial blood velocity at vessel wall must equal radial wall velocity
5. Repeat Step 1-4 until a stable solution is reached
6. $t = t + \Delta t$
7. Continue from Step 1

Finite elements

- Divide domain into parts
- Seek approximate solution over each part
- Assemble the parts





Continuous Galerkin finite element method

$$u(x,r) \approx u^e(x,r) = \sum_{j=1}^{n} U_j^e \psi_j^e(x,r)$$

$$\begin{aligned}\int \psi_i^e \nabla^2 u dV &= -\int \nabla\psi_i^e \cdot \nabla u dV + \oint \psi_i^e \cdot \nabla u ds \\ &= -\{U_j^e\} \int \nabla\psi_i^e \cdot \nabla\psi_j^e dV + \oint \psi_i^e \cdot \nabla u ds\end{aligned}$$

In PDE template operator form:

$$[\nabla^2](u) = -\{U_j^e\} \int \nabla\psi_i^e \cdot \nabla\psi_j^e dV = -[b2kk]\{U_j^e\}$$

⇨ [b2kk] =

X	X	X	X
X	X	X	X
X	X	X	X
X	X	X	X

Transformed Fluid Equations

To solve INS:

Use continuous Galerkin finite element method to approximate the equations

$$
\begin{aligned}
0 &= \int_{\Omega^e} \psi_i^e \{ \frac{\partial \sum_{j=1}^n U_j^e \psi_j^e}{\partial t} + \frac{1}{\rho} \frac{\partial \sum_{j=1}^n P_j^e \psi_j^e}{\partial r} - \nu (\frac{1}{r} \frac{\partial \sum_{j=1}^n U_j^e \psi_j^e}{\partial r} - \frac{\sum_{j=1}^n U_j^e \psi_j^e}{r^2}) \} dxdr \\
&+ \int_{\Omega^e} \nu (\frac{\partial \psi_i^e}{\partial x} \frac{\partial \sum_{j=1}^n U_j^e \psi_j^e}{\partial x} + \frac{\partial \psi_i^e}{\partial r} \frac{\partial \sum_{j=1}^n U_j^e \psi_j^e}{\partial r}) dxdr \\
&- \oint_{\Gamma^e} \nu \psi_i^e (\frac{\partial u}{\partial x} n_x + \frac{\partial u}{\partial r} n_r) ds \\
0 &= \sum_{j=1}^n \int_{\Omega^e} \psi_i^e \psi_j^e dxdr \frac{\partial W_j^e}{\partial t} + \sum_{j=1}^n \int_{\Omega^e} \frac{1}{\rho} \psi_i^e \frac{\partial \psi_j^e}{\partial x} dxdr P_j^e \\
&+ \sum_{j=1}^n \int_{\Omega^e} \nu \{ \frac{\partial \psi_i^e}{\partial x} \frac{\partial \psi_j^e}{\partial x} + (\frac{\partial \psi_i^e}{\partial r} - \frac{\psi_i^e}{r}) \frac{\partial \psi_j^e}{\partial r} \} dxdr W_j^e \\
&- \oint_{\Gamma^e} \nu \psi_i^e (\frac{\partial w}{\partial x} n_x + \frac{\partial w}{\partial r} n_r) ds
\end{aligned}
$$

$[M_e]\{DU_e\} + [C_e]\{P_e\} + [K_e]\{U_e\} = 0$

$[M_e]\{DW_e\} + [C_e]\{P_e\} + [K_e]\{W_e\} = 0$

Semi-discretization for Fluid Equations

$$u(x,r) \approx u^e(x,r) = \sum_{j=1}^{n} U_j^e \psi_j^e(x,r)$$

$$p(x,r) \approx p^e(x,r) = \sum_{j=1}^{n} P_j^e \psi_j^e(x,r)$$

$$w(x,r) \approx w^e(x,r) = \sum_{j=1}^{n} W_j^e \psi_j^e(x,r)$$

$$M_{ij}^e \;=\; \int_{\Omega^e} \psi_i^e \psi_j^e dxdr \;=\; DET_e[B200]$$

$$C_{ij}^e \;=\; \int_{\Omega^e} \frac{1}{\rho} \psi_i^e \frac{\partial \psi_j^e}{\partial r} dxdr \;=\; \frac{1}{\rho} DET_e[B20y]$$

$$K_{ij}^e \;=\; \int_{\Omega^e} \nu \{ \frac{\psi_i^e \psi_j^e}{r^2} + \frac{\partial \psi_i^e}{\partial x} \frac{\partial \psi_j^e}{\partial x} + (\frac{\partial \psi_i^e}{\partial r} - \frac{\psi_i^e}{r}) \frac{\partial \psi_j^e}{\partial r} \} dxdr$$

$$= \nu DET_e(\frac{1}{r^2}[b3000] + [b2kk] - \frac{1}{r}[b300y])$$

Method for Fluid Equations

- After using finite element method, Euler method and projection method are used.
- Euler forward method:

$$\frac{\partial u}{\partial t} = \frac{u^k - u^{k-1}}{\delta t}$$

- Projection method:

  - Use SPHI to replace pressure(p) and PHI to update SPHI

$$\{M^e\}\frac{u^k - u^{k-1}}{\delta t} + \{C^e\}\{SPHI^{k-1}\} + \{K^e\}\{U^k\} = 0$$

$$\{M^e\}\frac{w^k - w^{k-1}}{\delta t} + \{C^e\}\{SPHI^{k-1}\} + \{K^e\}\{W^k\} = 0$$

$$\nabla^2 PHI = \frac{u}{r} + \frac{\partial u}{\partial r} + \frac{\partial w}{\partial x}$$

$$SPHI^k = SPHI^{k-1} + PHI$$

1D Structure Equations

To solve Structure Equations :

1. Use continuous Galerkin finite element method

$$
\begin{aligned}
0 &= \int_{\Omega^e} \psi_i^e \{ M_0 \frac{\partial^2 \xi}{\partial t^2} + L_x \frac{\partial \xi}{\partial t} + K_x \xi - \frac{E_x h}{1-\sigma_\theta \sigma_x} \frac{\partial^2 \xi}{\partial x^2} - (\frac{E_x h \sigma_x}{a(1-\sigma_\theta \sigma_x)} + \frac{T_{t_0} - T_{\theta_0}}{a}) \frac{\partial \eta}{\partial x} \\
&- \mu [\frac{\partial w}{\partial r} + \frac{\partial u}{\partial x}]_a \} dx dr \\
0 &= \int_{\Omega^e} \psi_i^e \{ M_0 \frac{\partial^2 \eta}{\partial t^2} + L_r \frac{\partial \eta}{\partial t} + (K_r + \frac{E_\theta h}{a^2(1-\sigma_\theta \sigma_x)} - \frac{T_{\theta_0}}{a^2}) \eta - T_{t_0} \frac{\partial^2 \eta}{\partial x^2} \} dx dr \\
&+ \int_{\Omega^e} \psi_i^e \{ \frac{E_\theta h \sigma_\theta}{a(1-\sigma_\theta \sigma_x)} \frac{\partial \xi}{\partial x} - [p - 2\mu \frac{\partial u}{\partial r}]_a \} dx dr
\end{aligned}
$$

$$\{M^e\}\frac{\partial^2}{\partial t^2}\{X^e\}+\{C^e\}\frac{\partial}{\partial t}\{X^e\}+\{K^e\}\{X^e\}+\{D^e\}\{N^e\}=\{Q^e\}+\{S^e\}$$

$$\{M^e\}\frac{\partial^2}{\partial t^2}\{N^e\}+\{C^e\}\frac{\partial}{\partial t}\{N^e\}+\{K^e\}\{N^e\}+\{D^e\}\{X^e\}=\{Q^e\}+\{S^e\}$$

2. Use Newmark method to solve system of second order PDE

Newmark Method

This method involves equations of the form:

$$[M]\{\frac{\partial^2\eta}{\partial t^2}\} + [C]\{\frac{\partial\eta}{\partial t}\} + [K]\{\eta\} = F$$

The solution of this equation for the Newmark Method is :

$$\begin{aligned} & ([M] + \frac{\delta t}{2}[C] + \frac{\delta t^2}{4}[K])\{\frac{\partial^2\eta}{\partial t^2}\}_{n+1} \\ = \quad & [F]_{n+1} - [C](\{\frac{\partial\eta}{\partial t}\}_n + \frac{\delta}{2}\{\frac{\partial^2\eta}{\partial t^2}\}_n) - [K](\{\eta\}_n + \delta t\{\frac{\partial\eta}{\partial t}\}_n + \frac{\delta t^2}{4}\{\frac{\partial^2\eta}{\partial t^2}\}_n) \\ & \{\eta\}_{n+1} = \{\eta\}_n + \delta t\{\frac{\partial\eta}{\partial t}\}|_n + \frac{\delta t^2}{4}(\{\frac{\partial^2\eta}{\partial t^2}\}_n + \{\frac{\partial^2\eta}{\partial t^2}\}_{n+1}) \\ & \{\frac{\partial\eta}{\partial t}\}_{n+1} = \{\frac{\partial\eta}{\partial t}\}_n + \frac{\delta t}{2}(\{\frac{\partial^2\eta}{\partial t^2}\}_n + \{\frac{\partial^2\eta}{\partial t^2}\}_{n+1}) \end{aligned}$$

1D Version

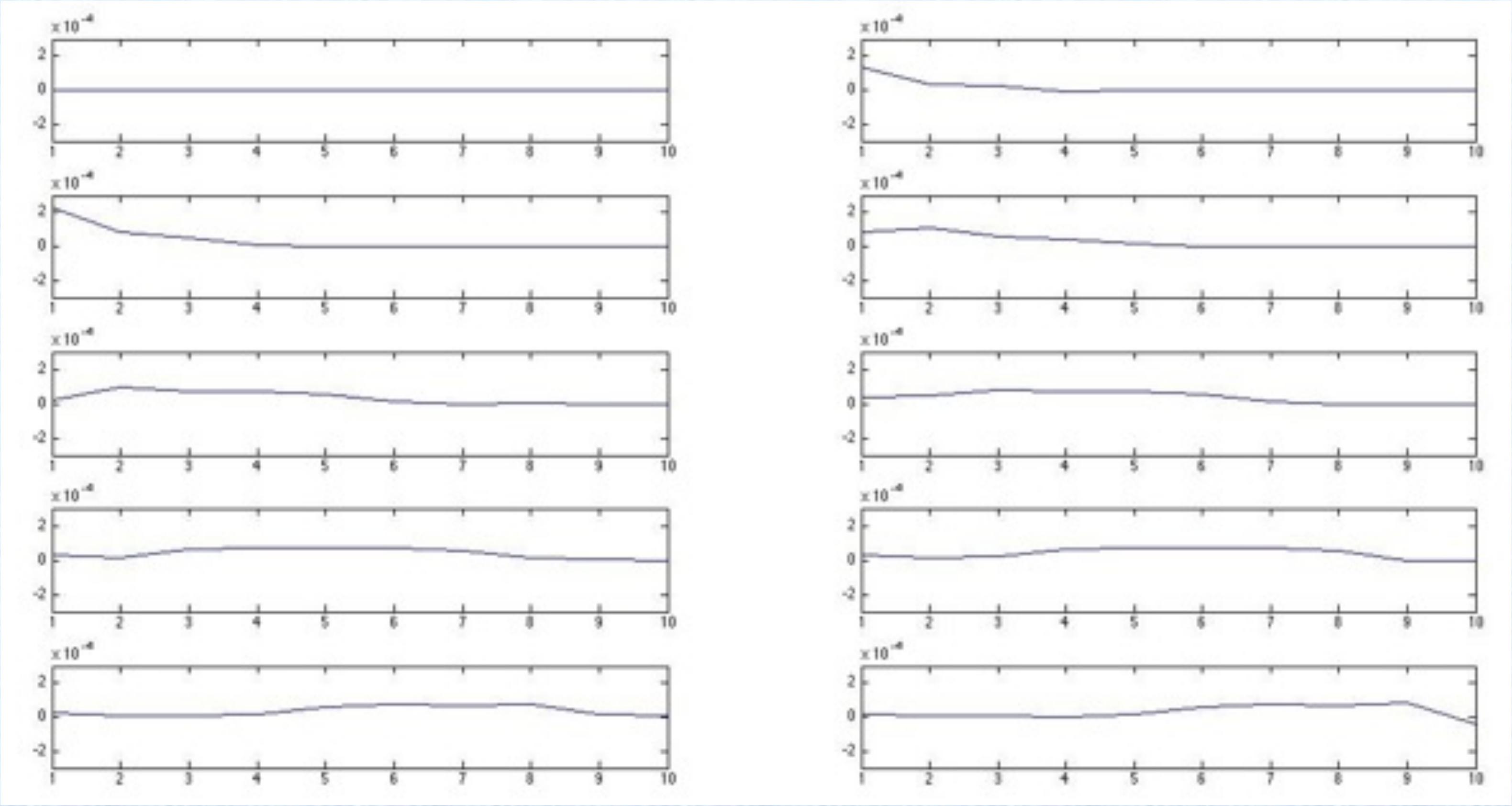
- serial code for 1D finite element method and Newmark method
- change X to DDX and N to DDN
- get full couple equations

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} DDX \\ DDN \end{pmatrix} = \begin{pmatrix} F1 \\ F2 \end{pmatrix}$$

- solve the above matrix by Lapack

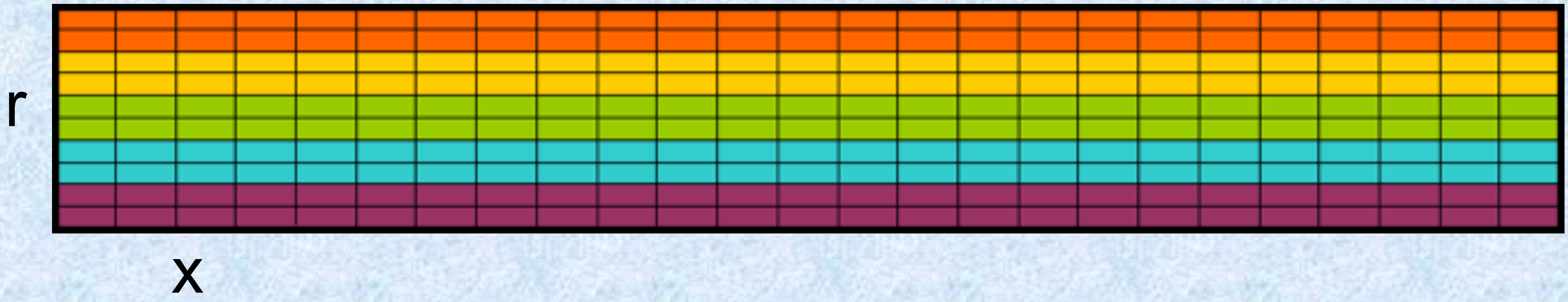
Benchmark Result

- Benchmark result of 1D vessel wall
- 1D serial code



Procedures for Fluid Equations

- darter, or star1
- Parallel Interoperable Computational Mechanics Simulation System (PICMSS)
- 5 processors
- Each responsible for several rows of grid
- 1cm diameter x 6cm length

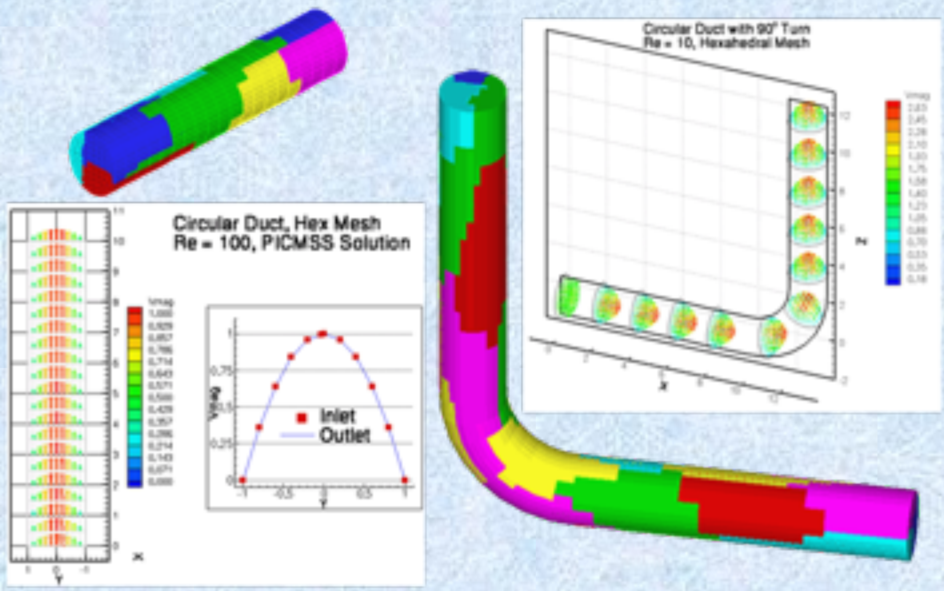


PICMSS

- parallel computational software
- solving equations with continuous Galerkin finite element method
- C program with MPI
- uses Trilinos iterative library for solving systems of linear equations generated internally by finite element method.
- 2D triangle and quadrilateral, and 3D tetrahedron and hexahedron master elements.
- fluid flow problems directly written in partial differential equation(PDE) template operator form.

Benchmark Results

- Benchmark result of fluid equations
- Inlet: all are 1 except boundary point
- blood vessel model: 1cm diameter x 6cm length
- Outlet:



2D axisymmetric structure equations

- Simulate the vessel wall with no tangential velocity
- Use the same structure equations on 3D mesh

$$M_0 \frac{\partial^2 \xi}{\partial t^2} + L_x \frac{\partial \xi}{\partial t} + K_x \xi$$

$$= \frac{E_x h}{1-\sigma_\theta \sigma_x} \frac{\partial^2 \xi}{\partial x^2} + \left(\frac{T_{t_0} - T_{\theta_0}}{a} - \frac{E_x h \sigma_x}{a(1-\sigma_\theta \sigma_x)}\right) \frac{\partial \eta}{\partial x} - \mu\left[\frac{\partial w}{\partial r} + \frac{\partial u}{\partial x}\right]_a$$

$$M_0 \frac{\partial^2 \eta}{\partial t^2} + L_r \frac{\partial \eta}{\partial t} + K_r \eta$$

$$= T_{t_0} \frac{\partial^2 \eta}{\partial x^2} + \left(\frac{T_{\theta_0}}{a^2} - \frac{E_\theta h}{a^2(1-\sigma_\theta \sigma_x)}\right)\eta + \frac{E_\theta h \sigma_\theta}{a(1-\sigma_\theta \sigma_x)} \frac{\partial \xi}{\partial x} + \left[p - 2\mu \frac{\partial u}{\partial r}\right]_a$$

- Use PICMSS to solve

2D axisymmetric structure equations(PICMSS)

```
  *

 OPERATORS  4
OP_1   * cn200 *
OP_2   * cn2xx *
OP_3   * cn20x *
OP_4   * cn10 *

NUMBER_OF_SETS  5

DDUDDV_EQUATION_SET   0:

   OPERATORS  4
   OP_1 OP_2 OP_3 OP_4

  EQUATIONS 2

   RHS_DDU  15
   mCKU1 OP_1 DDU
   MKU2 OP_2 DDU
   DCUDT2 OP_3 DDV
   DCU OP_3 VL
   DCUDT OP_3 DVL
   DCUDT2 OP_3 DDVL
   MSU OP_4 1
   C OP_1 DUL
   CDT OP_1 DDUL
   KU1 OP_1 UL
   KU2 OP_2 UL
   KU1DT OP_1 DUL
   KU2DT OP_2 DUL
   KU1DT2 OP_1 DDUL
   KU2DT2 OP_2 DDUL
```

```
ineqnt.indat                                20,1          19%
```

```
   KU2DT2 OP_2 DDUL

   RHS_DDV  11
   mCKV OP_1 DDV
   DVDT2 OP_3 DDU
   DCV OP_3 UL
   DCVDT OP_3 DUL
   DCVDT2 OP_3 DDUL
   MSV OP_4 1
   C OP_1 DVL
   CDT OP_1 DDVL
   KV OP_1 VL
   KVDT OP_1 DVL
   KVDT2 OP_1 DDVL

  JAC_DDU_by_DDU  2
  mCKU1 OP_1
  MKU2 OP_2

  JAC_DDU_by_DDV  1
  DCUDT2 OP_3

  JAC_DDV_by_DDU  1
  DVDT2 OP_3

  JAC_V_by_V  1
  mCKV OP_1

  NO_NEU_BC_TYPE_U 0

  NO_NEU_BC_TYPE_V 0

U_EQUATION_SET  1:
```

```
ineqnt.indat                                67,1          53%
```

Full 3D Fluid Equations

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)+\rho g_x$$

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)+\rho g_y$$

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)+\rho g_z.$$

3D structure Equations

- Use the approach from Raoul et al. [3]
- *D* is the deformation of vessel wall, and *p* is the pressure of the wall

$$\frac{\partial}{\partial x_1}(F_{11}^2+F_{12}^2-1-p)+\frac{\partial}{\partial x_2}(F_{21}F_{11}+F_{22}F_{12})=0$$

$$\frac{\partial}{\partial x_1}(F_{21}F_{11}+F_{22}F_{12})+\frac{\partial}{\partial x_2}(F_{21}^2+F_{22}^2-1-p)=0$$

$$-\frac{\partial p}{\partial x_3}=0$$

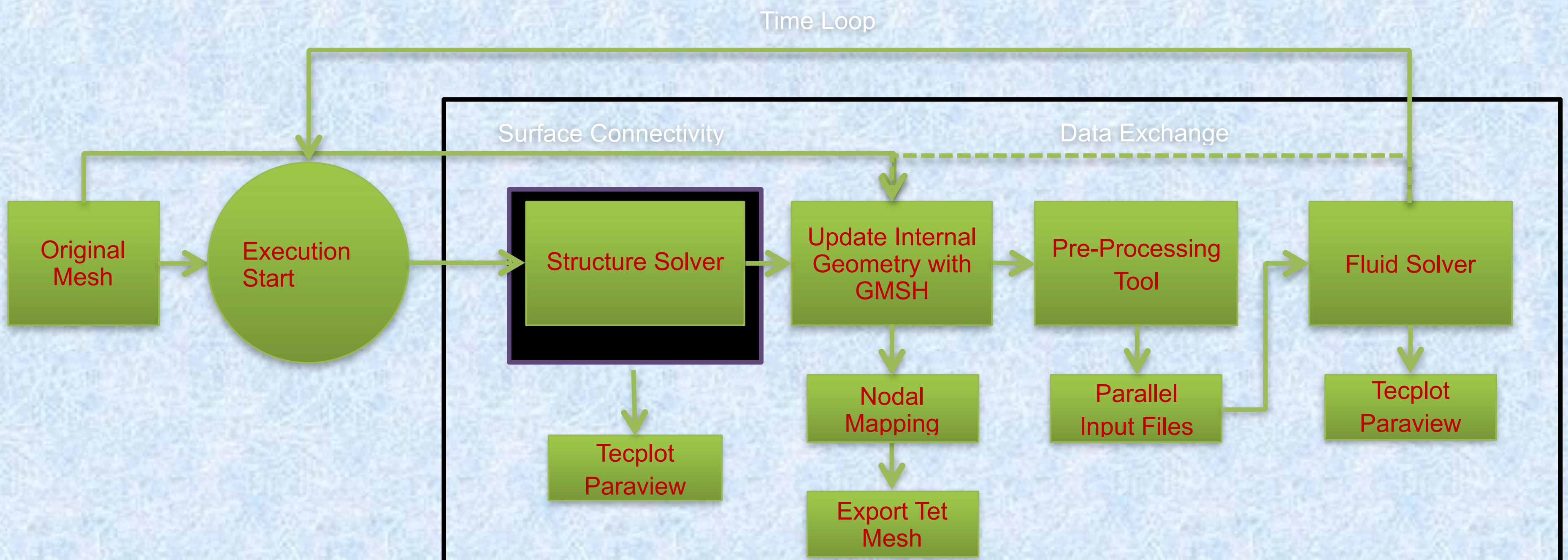
$$F_{11}F_{22}-F_{21}F_{12}=0$$

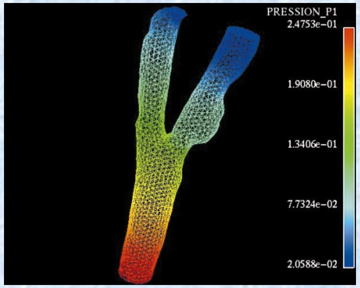
$$F_{ij}=\frac{\partial D_i}{\partial x_j}$$

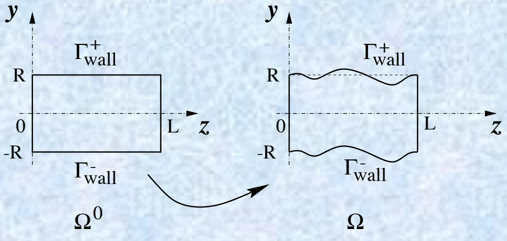
DIEL

- Multi-physics problems combining multiple sets of governing principles and conditions in a variety of medium
- Physical domains or conditions are separated and computed independently
- Interaction occurs through a set of shared boundary points, weak coupling
- Reduces the complexity of the system
- Can be solved efficiently on a parallel computer

Workflow Using DIEL







Future Plans

- Run the code of 2D axisymmetric structure equations on PICMSS and compare with result of 1D serial code
- Solve full 3D fluid equations and structure equations
- Solve fully coupled fluid-structure equations
- Use DIEL to solve coupled equations

Acknowledgements

- Mentors: Kwai Wong
- And other JICS staff

Reference:

[1] : Quarteroni, Alfio; Tuveri, Massimiliano; Veneziani, Alessandro. “Computational vascular fluid dynamics: problems, models, and methods" Comput Visual Sci 2:163-197 (2000).

[2] : *Johnny T. Ottesen, Mette S. Olufsen, Jesper K. Larsen, “Applied Mathematical Models in Human Physiology (Siam Monographs on Mathematical Modeling and Computation)." SIAM, 2004.

[3] : Raoul van Loon, Patrick D. Anderson, Frank P.T. Baaijens, Frans N. Van de Vosse, “A three-dimensional fluid-structure interaction method for heart valve modelling”, C. R. Mecanique 333 (2005)