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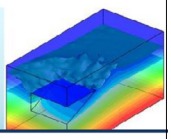
SEOUL NATIONAL UNIVERSITY OF SCIENCE & TECHNOLOGY

Computational Fluid Dynamics Lab
Department of Mechanical Engineering



"다중의료영상을 활용한 3차원 초정밀 시뮬레이션 기반 심혈관 질환 진단-치료 통합소프트웨어 시스템 개발"

유체-구조 상호작용을 고려한 혈류유동 해석의 고속연산기법

전병진[1], Ha Truong Sang[2], 최형권[3], 이상욱[4], 장혁재[5]

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4) 울산대학교, 기계공학과
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발표자 : 최형권 교수

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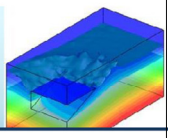
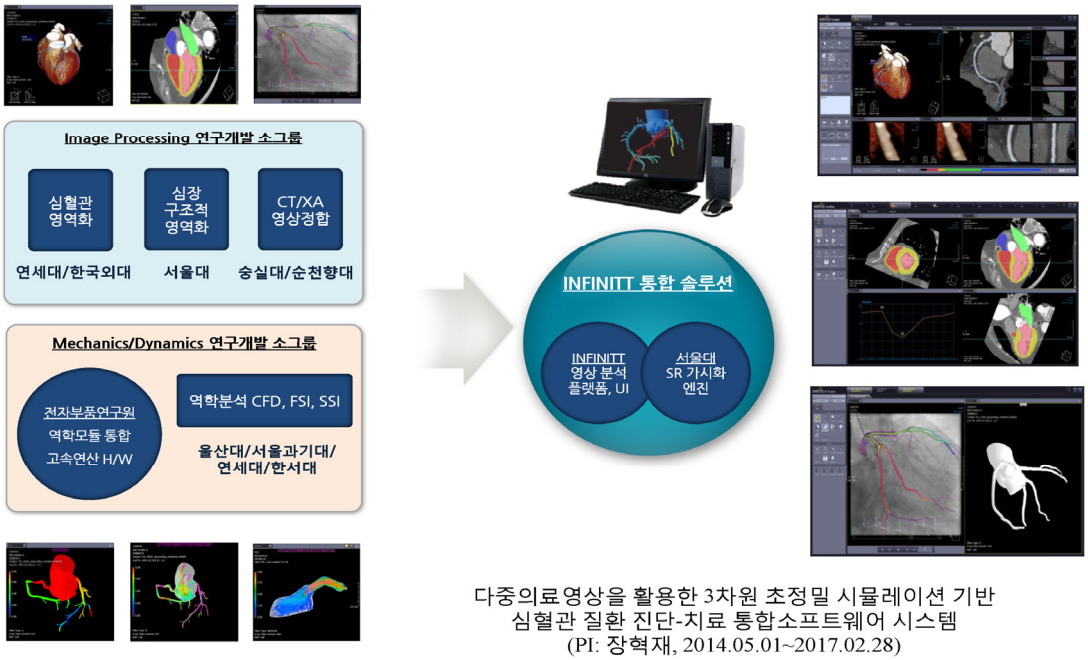


유체-구조 상호작용(FSI)을 고려한 혈류유동 해석의 고속연산기법

- **FSI 선행연구 및 고속화 연산 기법 소개**
- **고속화 연산 기법을 이용한 수치해석 결과**
- **초고속 연산을 위한 FSI 알고리즘의 병렬화**
- **임상 해석 결과**

Background



다중의료영상을 활용한 3차원 초정밀 시뮬레이션 기반
심혈관 질환 진단-치료 통합소프트웨어 시스템
(PI: 장혁재, 2014.05.01~2017.02.28)

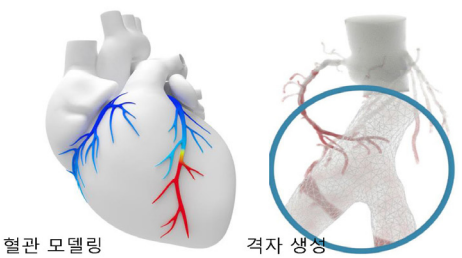
Previous studies

- 타 연구와의 차별성

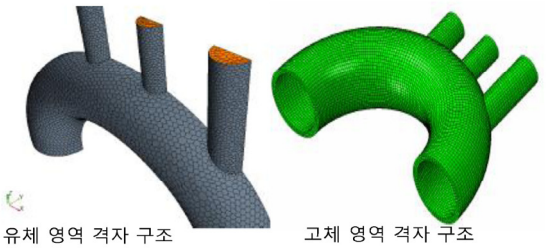
1) Heart flow : 유동 해석을 통해 FFR 값 도출 (기존 타 연구 방법과 동일)

2) Siemens (STAR-CCM + Abaqus) : 유체-구조 상호작용 해석 시간에 대한 언급이 없음

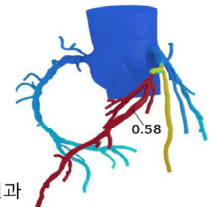
3) Ansys (Mechanical + Fluent) : 본 개발 코드에 비해서 단일 코어를 이용한 해석 시간이 15배 이상 느림



혈관 모델링 격자 생성

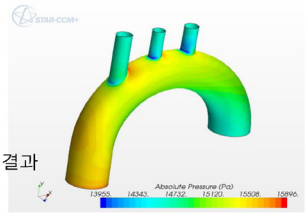


유체 영역 격자 구조 고체 영역 격자 구조



FFR 수행 결과

[Heart flow] 유동 해석 결과



압력 분포 결과

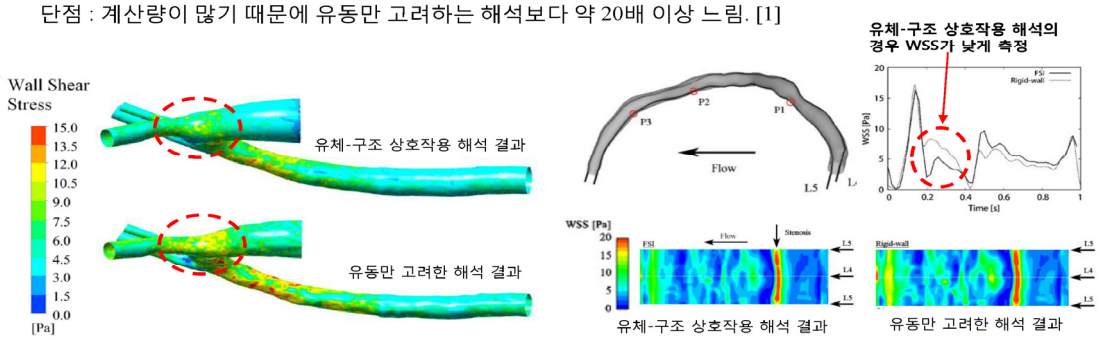
[Siemens] 유체-구조 상호작용 해석 결과

Previous studies

- 유체-구조 상호작용 해석의 중요성

장점 : 1) 혈관의 움직임을 고려함 2) 다양한 파열 예측 인자를 얻을 수 있음.

단점 : 계산량이 많기 때문에 유동만 고려하는 해석보다 약 20배 이상 느림. [1]

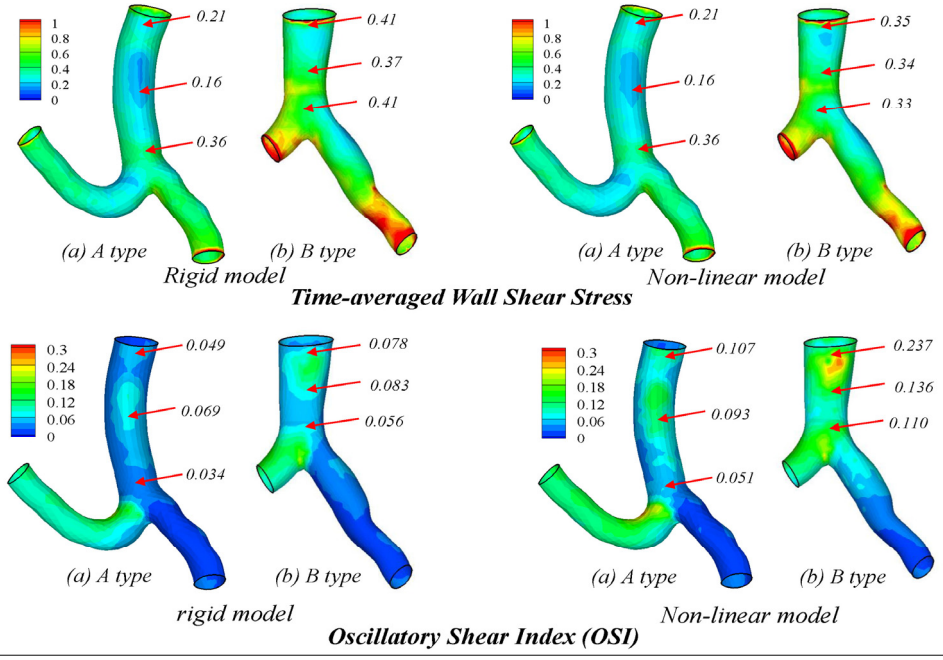


유체-구조 상호작용 해석 유무에 따른 벽전단응력 결과 비교[1],[2]

[1] A.G. Brown et al., "Accuracy vs. computational time : Translating arotic simulations to the clinic", Journal of Biomechanics, Vol. 45, pp. 516-523, 2012.
[2] R. Torii et al., "Fluid-structure interaction analysis of a patient-specific right coronary artery with physiological Velocity and pressure waveforms", Communications in Numerical Methods in Engineering, Vol. 25, pp. 565-580, 2009.

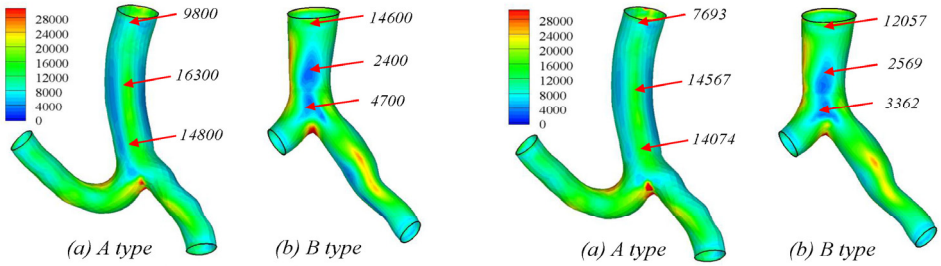
Previous studies

✓ Comparison of rigid and non-linear FSI model

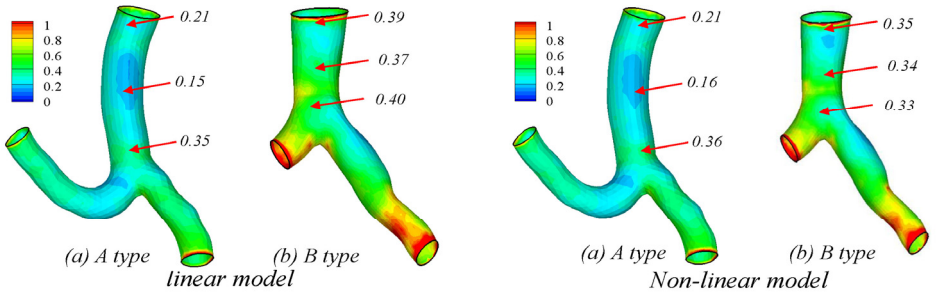


Previous studies

✓ Comparison of linear and non-linear FSI model



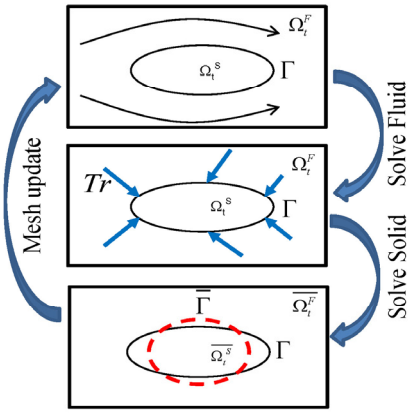
Time-averaged Von-mises Stress

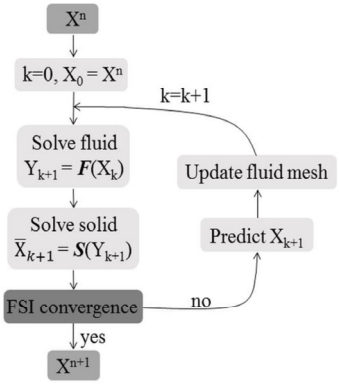


Time-averaged Wall Shear Stress

Partitioned method solving Fluid-Structure Interaction problems

Partitioned (staggered) method => Iteration algorithm is used





Flow chart of FSI algorithm

Denote: $\mathbf{X}_k$ *is predict value of variables on interface (displacement)* at *kth*-(FSI) iterations of time level *n-th*

The solution after solving FSI

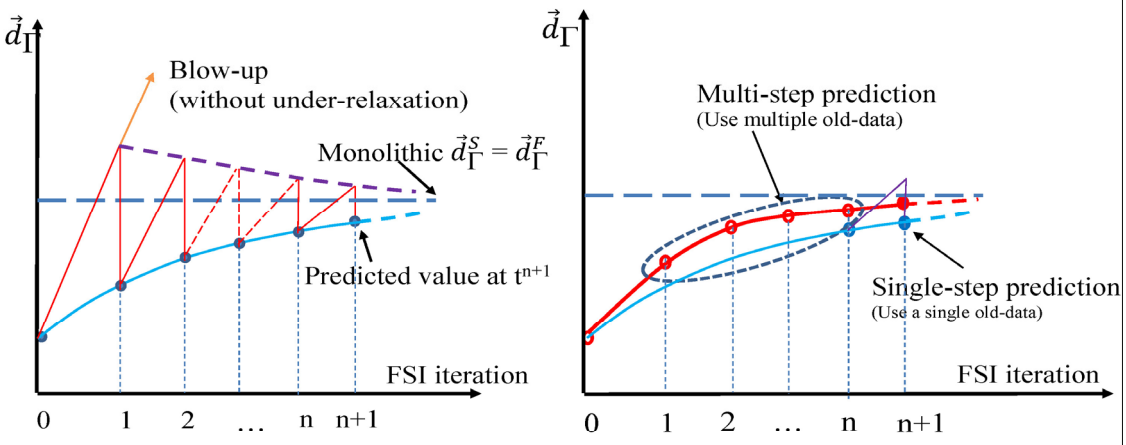
$\overline{\mathbf{X}}_{k+1} = \mathbf{S}^{\circ}\mathbf{F}\,(\mathbf{X}_k)$;

FSI Error $\mathbf{r}_k = \overline{\mathbf{X}}_{k+1} - \mathbf{X}_k$

If $\|\mathbf{r}_k\| < \varepsilon \Rightarrow$ ***FSI*** *convergence* $\Rightarrow$ *exit*

Otherwise predict $\mathbf{X}_{k+1}$ *for next FSI iteration*

Partitioned method solving Fluid-Structure Interaction problems



Partitioned method solving Fluid-Structure Interaction problems

The formulations

1- Fixed relaxation $\mathbf{X}^{k+1} = \omega * \bar{\mathbf{X}}^{k+1} + (1\text{-}\omega)*\mathbf{X}^k$

Or $\mathbf{X}^{k+1} = \mathbf{X}^k + \underbrace{\omega*\mathbf{r}^{k+1}}_{\text{Increment}}$ Where $\mathbf{r}^{k+1} = \bar{\mathbf{X}}^{k+1} - \mathbf{X}^k$

$\mathbf{X}^k$: predict value of current iteration
$\bar{\mathbf{x}}^{k+1}$: Solution of current iteration: $\bar{\mathbf{X}}^{k+1} = \mathbf{S}\circ\mathbf{F}(\mathbf{X}^k)$
$\mathbf{X}^{k+1}$: predict value for next iteration

2- Aitken's relaxation (adaptive relaxation) [1] $\omega_{k+1} = -\omega_k \dfrac{(\mathbf{r}^k)^{\mathrm{T}}(\mathbf{r}^{k+1} - \mathbf{r}^k)}{\left|\mathbf{r}^{k+1} - \mathbf{r}^k\right|^2}$

$\mathbf{X}^{k+1} = Function\ (\bar{\mathbf{X}}^{k+1}, \bar{\mathbf{X}}^k, \mathbf{X}^k, \mathbf{X}^{k-1})$

3- QN_ILS [2] : Quasi-Newton with Inverse Jacobian from a Least-Squares model

$$\mathbf{X}^{k+1} = \mathbf{X}^k + \underbrace{\textstyle\sum_{i=1,k-1} \Delta\bar{\mathbf{X}}^{i+1} * c^i + \mathbf{r}^{k+1}}_{\text{Increment}}$$

Denote: $\Delta\bar{\mathbf{X}}^{i+1} = \bar{\mathbf{X}}^{i+1} - \bar{\mathbf{X}}^{k+1}$

c^i can be predicted such that the error $\mathbf{r}^{k+2}$ is minimum

[1] Ulrich Küttler et al, 2008, Fixed-point fluid–structure interaction solvers with dynamic relaxation.
[2] Joris Degroote et al, 2010 , Performance of partitioned procedures in fluid–structure interaction. Computers and Structures Vol.88, p.446-457.

Partitioned method solving Fluid-Structure Interaction problems

Least squares method

Using least squares method to determined c^i

$$\left\| \mathbf{r}^{k+1} + \sum_{i=1,k-1} \Delta\mathbf{r}^i * c^i \right\|_2 \text{ is minimum} \Leftrightarrow \{[\Delta\mathbf{r}]^T[\Delta\mathbf{r}]\} * c^i = [\Delta\mathbf{r}]^T(-\mathbf{r}^k)$$

Or $[\mathbf{A}]*\mathbf{C} = \mathbf{B}$

$$\Delta\mathbf{r} = \begin{pmatrix} n_{eq\Gamma} \times n_{step} \end{pmatrix} \Rightarrow [\mathbf{A}] = [\Delta\mathbf{r}]^T[\Delta\mathbf{r}] = \begin{pmatrix} n_{step} \times n_{step} \end{pmatrix}$$

$$\mathbf{B} = [\Delta\mathbf{r}]^T(-\mathbf{r}^{k+1})$$

With $n_{step} < 50$

Partitioned method solving Fluid-Structure Interaction problems

Implementation

Prediction of $\mathbf{X}^{k+1}$ by using n_{step} previous FSI iteration

1- Solve FSI at *k-th* iteration $\overline{\mathbf{X}}^{k+1} = \mathbf{S}\circ\mathbf{F}(\mathbf{X}^k)$

2– Calculate $\mathbf{r}^i = \overline{\mathbf{X}}^{i+1} - \mathbf{X}^i$, i=1, k

2- Calculate $\Delta\overline{\mathbf{X}}^{i+1} = \overline{\mathbf{X}}^{i+1} - \overline{\mathbf{X}}^{k+1}$, i=1,k-1

3- Calculate $\Delta\mathbf{r}^i = \mathbf{r}^i - \mathbf{r}^k$, i=1, k-1,

=> construct matrix $[\Delta\mathbf{r}] = [\Delta\mathbf{r}^1, \Delta\mathbf{r}^2 \ldots \Delta\mathbf{r}^{k-1}]$

4- Calculated matrix **A** and vector **B** follow: $\mathbf{B} = [\Delta\mathbf{r}]^T(-\mathbf{r}^k)$

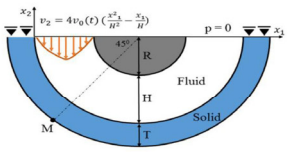
$[\mathbf{A}] = [\Delta\mathbf{r}]^T[\Delta\mathbf{r}]$

5- Solve $[\mathbf{A}]*\mathbf{C} = \mathbf{B}$ to find c^i

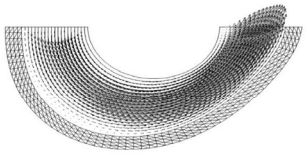
6- Calculate prediction value $\mathbf{X}^{k+1} = \sum_{i=1,k-1} \Delta\overline{\mathbf{X}}^{i+1} * c^i + \overline{\mathbf{X}}^{k+1}$

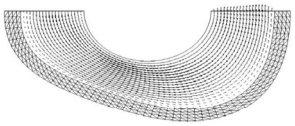
Application for simulating blood vessel

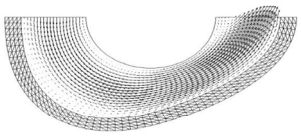
2D flow in a circular channel



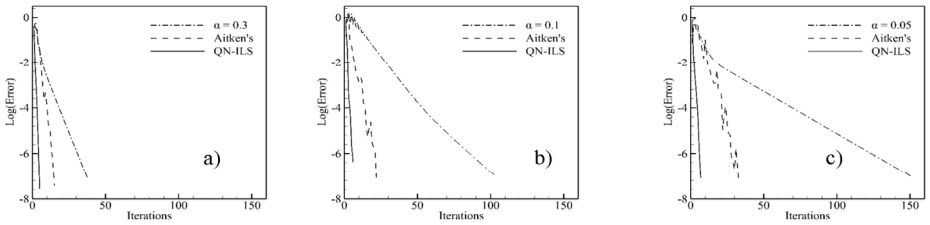
Schematic of the flow in a circular channel







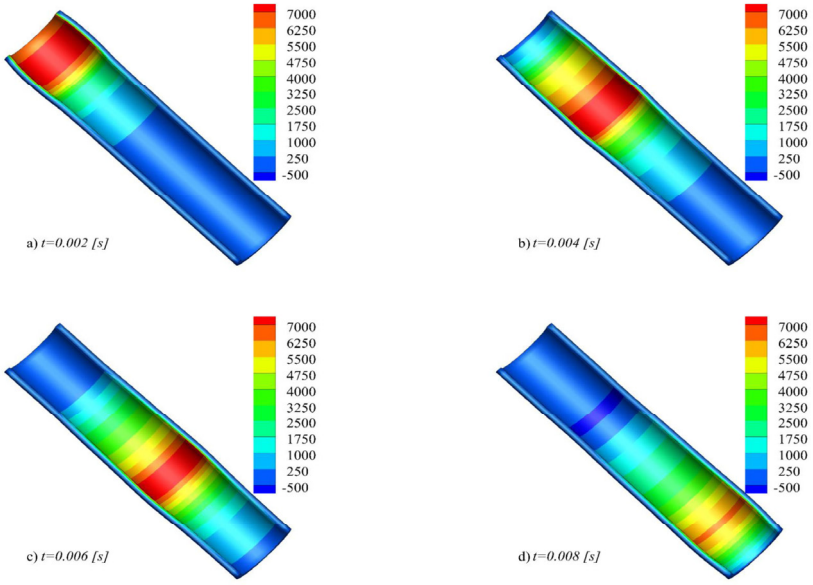
b) $time = 2.4\ s$



The history of convergence a) $\bar{\rho} = 10$, b) $\bar{\rho} = 1.2$, c) $\bar{\rho} = 0.5$

Application for simulating blood vessel

Flow in 3D straight flexible tube



a) *t=0.002 [s]*

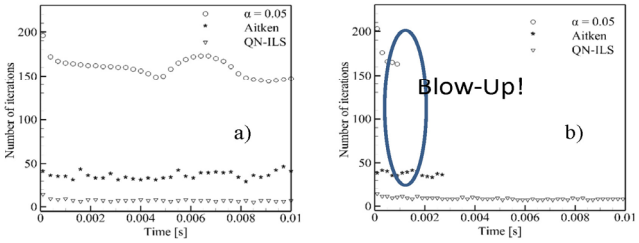
b) *t=0.004 [s]*

c) *t=0.006 [s]*

d) *t=0.008 [s]*

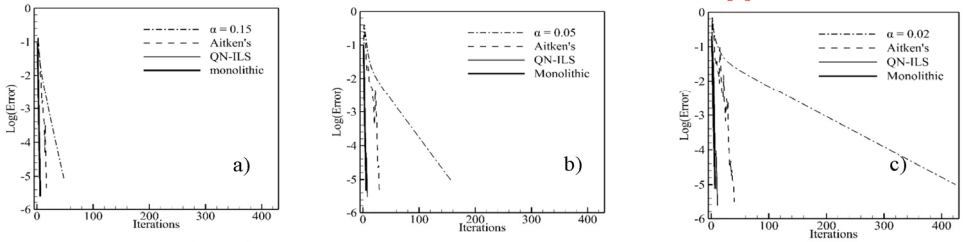
Application for simulating blood vessel

Flow in 3D straight flexible tube



The number of FSI coupling versus time;
a) small displacement, b) large displacement

- The QN-ILS is much faster than others
- In large displacement case: fixed under-relaxation and Aitken's were divergence.
- With the heavy solid ($\bar{\rho} = 10$) there are not big different of partitioned methods in term of convergence behaviour
- With same density case($\bar{\rho} = 1.2$): QN-ILS is much faster than others methods
- With slight solid ($\bar{\rho} = 0.5$): Fixed-relaxation very poor.
- QN_ILS is comparable with monolithic method [3]

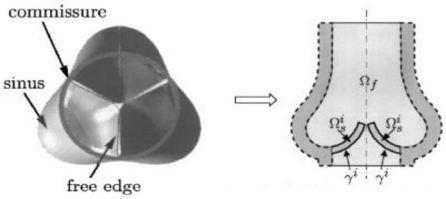


The history of convergence a) $\bar{\rho} = 10$, b) $\bar{\rho} = 1.2$, c) $\bar{\rho} = 0.5$

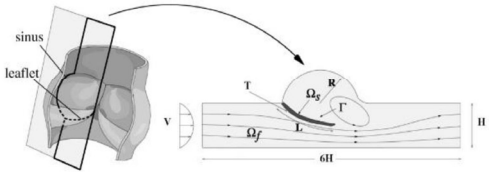
[3] S. Kang et al, 2012 , Investigation of fluid–structure interactions using a velocity-linked P2/P1 finite element method and the generalized- a method, International Journal for Numerical Methods in Engineering, vol. 90, pp:1539-1547.

Application for simulating blood vessel

Flow through the aortic valves



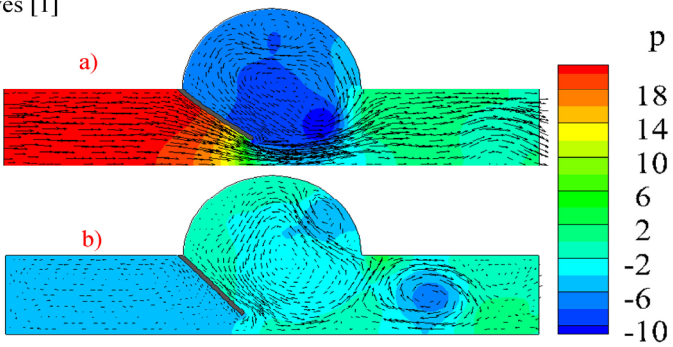
Geometry of the aortic valves [1]



2D simulation

Parameter	
Radius	R= H = 20 mm
Length	L = 20 mm
Young modulus	E = 1.E6 Pa
Poisson ratio	0.4
Density	$\rho_F = \rho_F$=1000 *kg/m3*

Pulsatile velocity was set at inlet,
the maximum Re = 250,
Time simulation T=1.0s

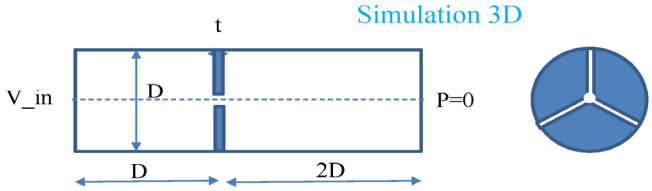


Velocity field and pressure contour at
a) time = T/2 and b) time = T

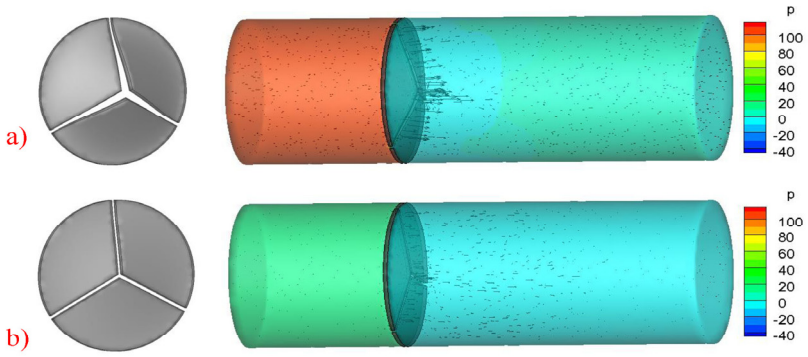
Application for simulating blood vessel

Flow through the aortic valves

Simulation 3D

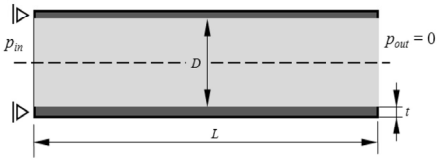


t = 1 mm
D = 40 mm



The valves opening and fluid flow at: a) time = T/2, b) time = T

Application for simulating blood vessel



Flexible pipe configuration

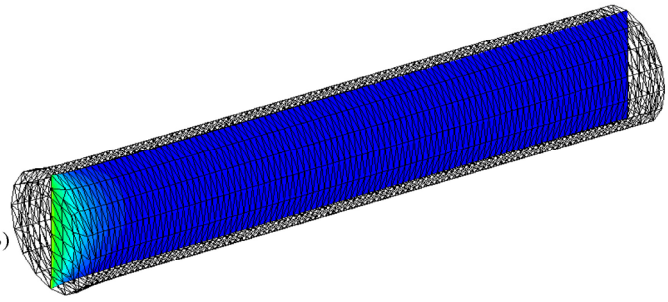
Geometry		
$L = 0.1\ m$	$D = 0.02\ m$	$t = 0.002\ m$

Material properties			
Fluid	$\rho_f = 1000\ kg/m^3$	$\mu = 0.004\ Pa.s$	
Solid	$\rho_s = 1000\ kg/m^3$	$E = 1.0e6\ Pa$	$\nu = 0.3$

Performance of ANSYS and partitioned in-house code

CPU time for 80 time-steps	
Solvers	Time
ANSYS	12.28 (hours)
QN_ILS	0.85 (hours)

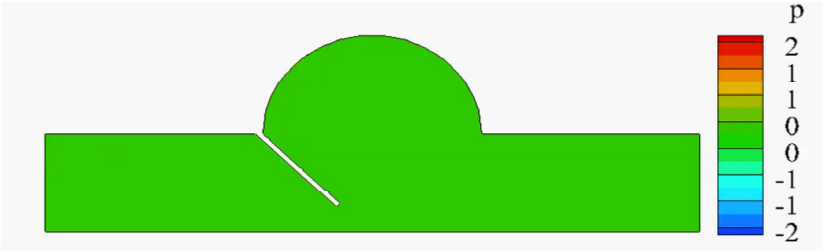
The in-house code, QN_ILS method is around 15 times faster than the commercial code (ANSYS)



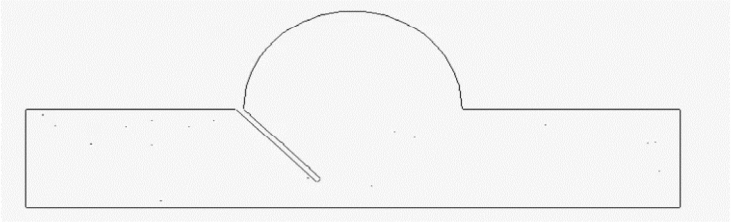
Application for simulating blood vessel

2D animation

Pressure contour

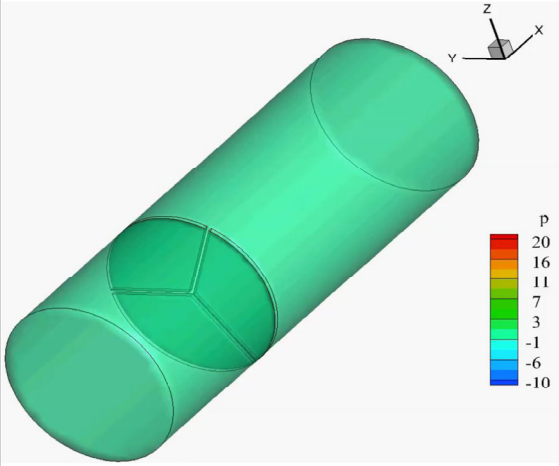


Velocity field

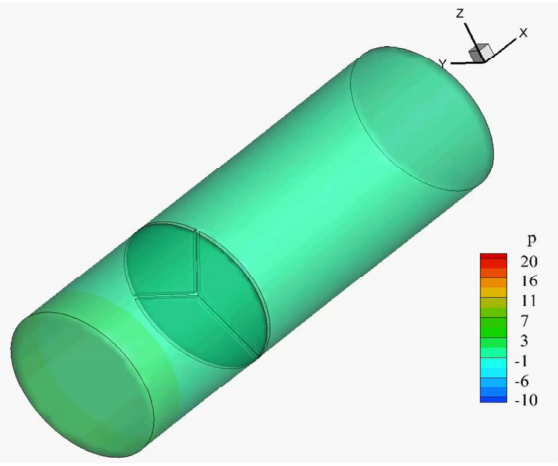


Application for simulating blood vessel

3D flow through aortic valves



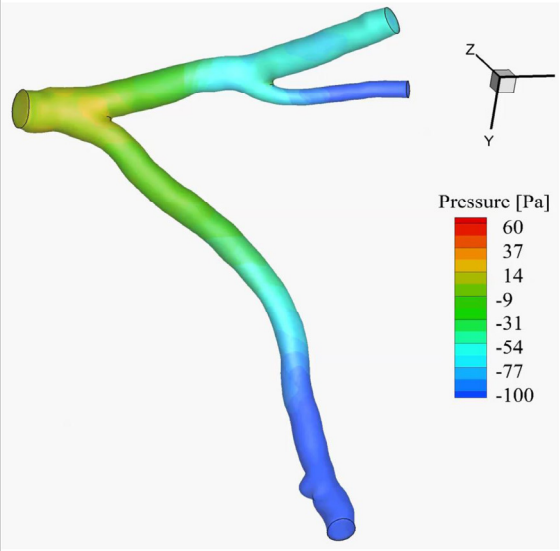
Elastic valves



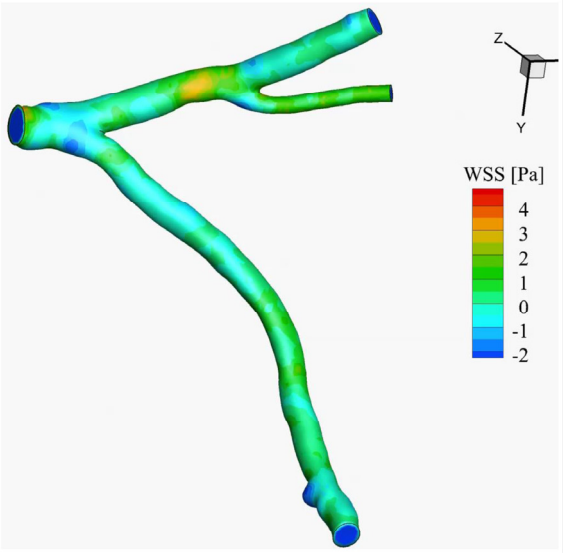
Rigid valves

Application for simulating blood vessel

3D flow through coronary



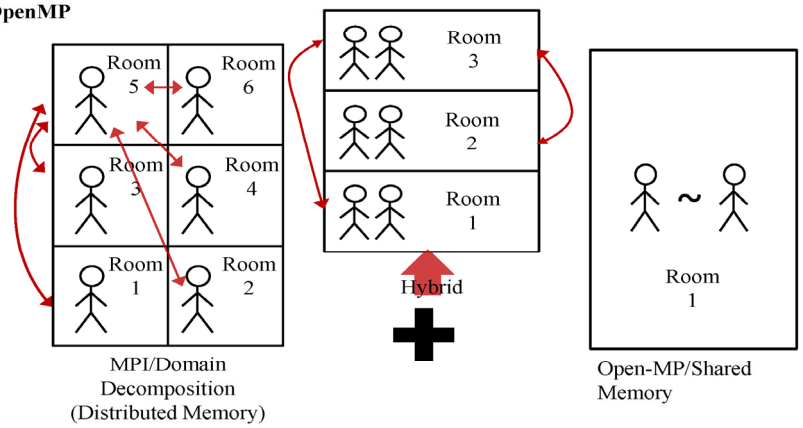
Pressure contour

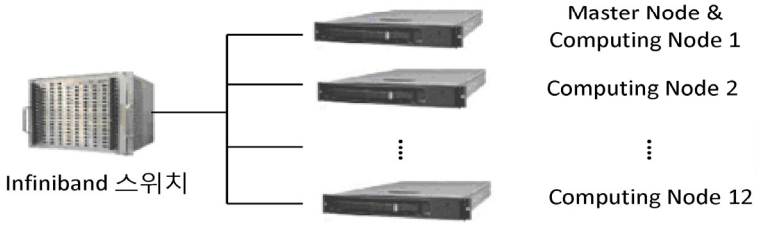


Wall shear stress contour

Parallelization

- MPI vs. OpenMP





프로세서	Intel Xeon E5-2680 V2 2.80GHz Cache size : 25MB
코어	240개 (1node : 20개)

Parallelization

- MPI vs. OpenMP

MPI/Distributed memory

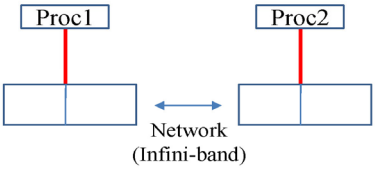
```
Do # 1~Nd/Proc
  tmp=tmp+x(ja(i))*au(i)
ENDDO
```

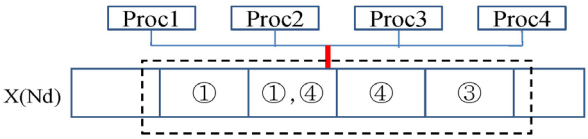
Each Processor execute
'Do sentence' independently.

Open-MP/Shared Memory

```
$OMP PARALLEL DO
Do # j=1~Nd(/proc)
    tmp=tmp+x(ja(i))*au(i)
ENDDO
```

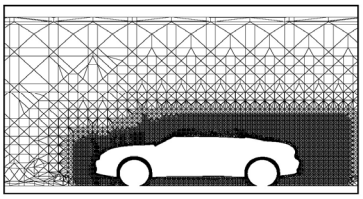
Many processor execute
'Do sentence' together.
(in the sense of 'memory access')

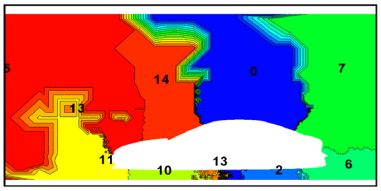


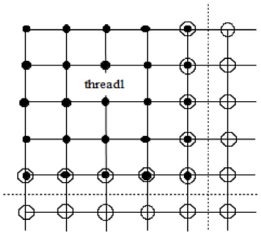


Parallelization

- Parallel Conjugate Gradient(PCG) $Ax = f \rightarrow r = Ax - f$



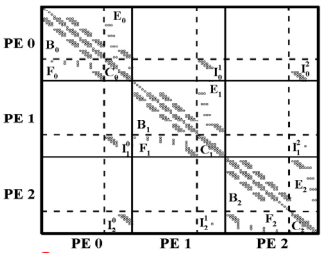




Mesh Partition by METIS Library
↓
Local Matrix Generation
↓
Solution by Parallel Preconditioned Conjugate Gradient Method

Communication by Message Passing Interface Library

Parallel Preconditioning by Block ILU(0)



1. $\alpha_j = \dfrac{\{z_j\}^T \{r_j\}}{\{d_j\}^T [A] \{d_j\}}$

2. $\{x_{j+1}\} = \{x_j\} + \alpha_j \{d_j\}$

3. $\{r_{j+1}\} = \{r_j\} - \alpha_j [A] \{d_j\}$

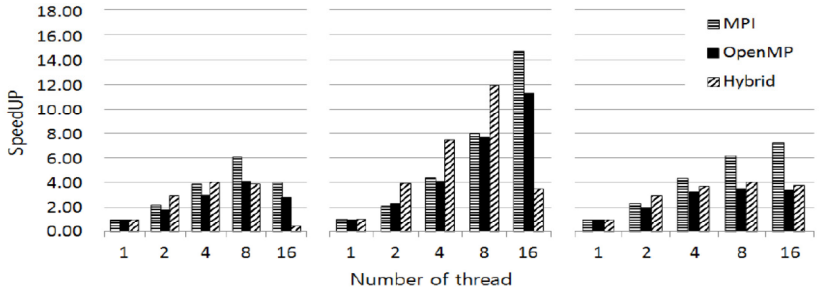
4. $\{z_{j+1}\} = [M]^{-1} \{r_{j+1}\}$

5. $\beta_j = \dfrac{\{z_{j+1}\}^T \{r_{j+1}\}}{\{z_j\}^T \{r_j\}}$

6. $\{d_{j+1}\} = \{z_{j+1}\} + \beta_j \{d_j\}$

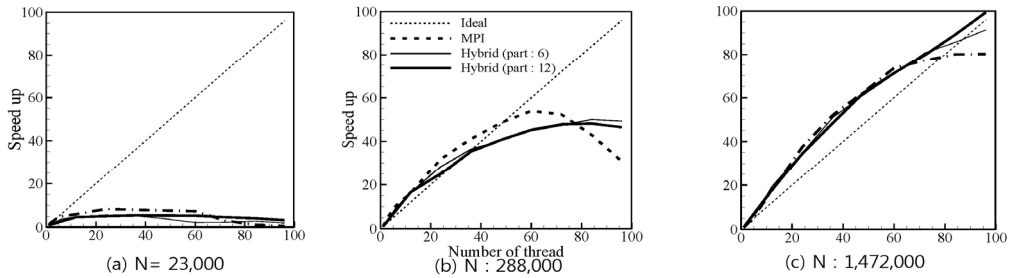
Parallelization

- 공유 메모리 시스템에서의 병렬 성능 비교 결과



(a) N=23,000 (b) N=144,000 (c) N=1,472,000

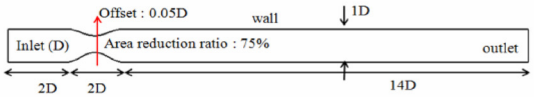
- 분산 메모리 시스템에서의 병렬 성능 비교 결과



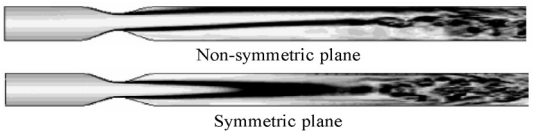
(a) N= 23,000 (b) N : 288,000 (c) N : 1,472,000

Parallelization

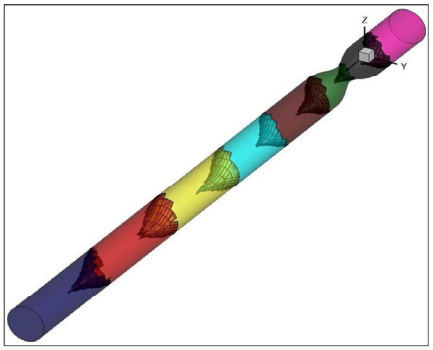
- METIS를 이용한 영역분할 결과 및 병렬 성능 (협착관 유동 해석)

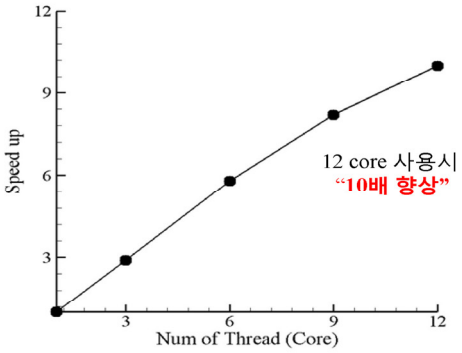


Schematic of the eccentric stenosis model



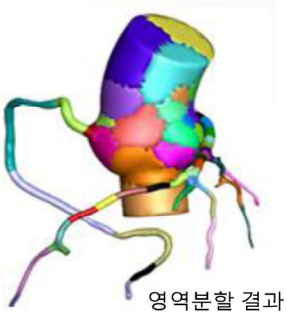
Instantaneous vorticity magnitude contours
Node : 320,000



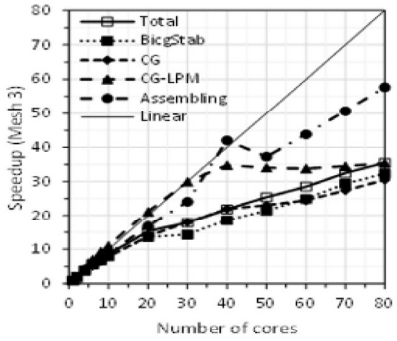


Parallelization

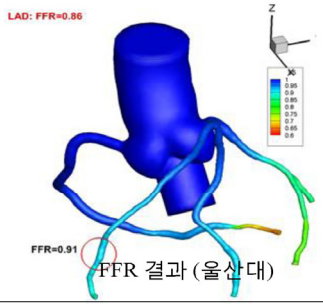
- METIS를 이용한 영역분할 결과 및 병렬 성능 (관상동맥 해석)



영역분할 결과



격자 생성 (한서대)



FFR 결과 (울산대)

관상동맥 시뮬레이션
"20분 이내 완료"

Parallelization

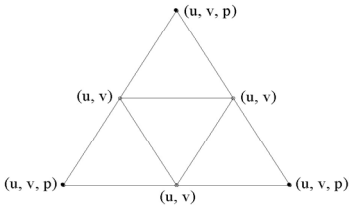
- 유체 영역에 대한 병렬화 수행

- Three-step splitting method based on P2P1 finite element method

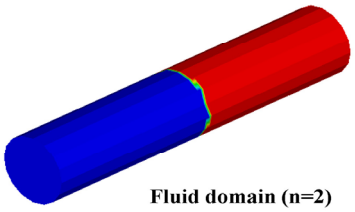
$$\frac{\hat{u}_i - u_i^n}{\Delta t} + \frac{1}{2}\left(\hat{u}_j \hat{u}_{i,j} + u_j^n u_{i,j}^n\right) = -\frac{1}{\rho} p^n{}_{,i} + \frac{1}{2}\left(\hat{\tau}_{ij} + \tau_{ij}^n\right)_{,j} + S_i^n$$

$$\frac{u_i^* - \hat{u}_i}{\Delta t} = \frac{1}{\rho} p^n{}_{,i}$$

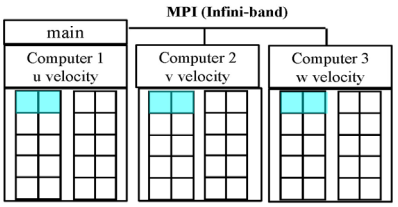
$$\begin{cases} \dfrac{u_i^{n+1} - u_i^*}{\Delta t} = -\dfrac{1}{\rho} p_{,i}^{n+1} \\ u_{i,i} = 0 \end{cases}$$



- Parallelization : METIS + MPI

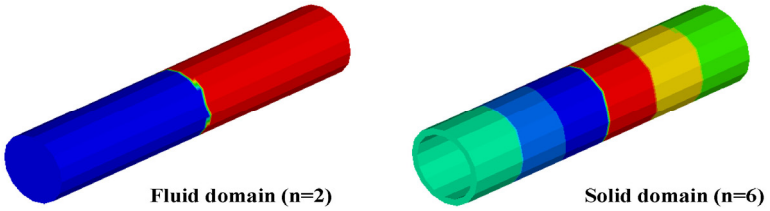


Fluid domain (n=2)

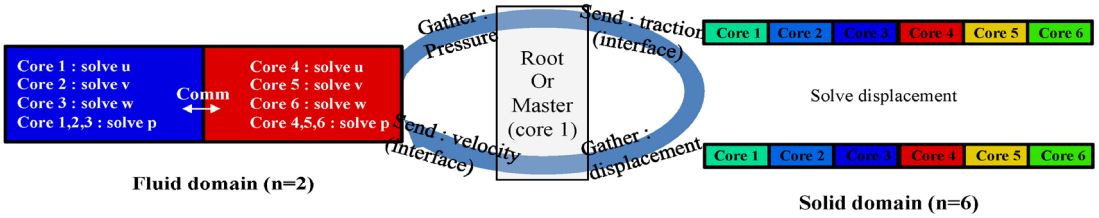


Parallelization

- 자동영역분할 알고리즘(METIS)를 이용한 결과

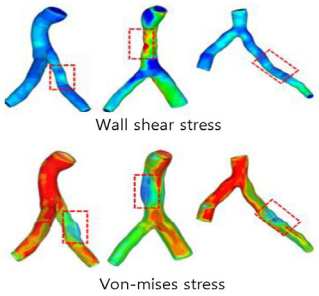


- 분리 알고리즘의 병렬 연산 과정 : 영역분할 + MPI



Parallelization

- 알고리즘 최적화에 따른 계산 속도의 개선 결과

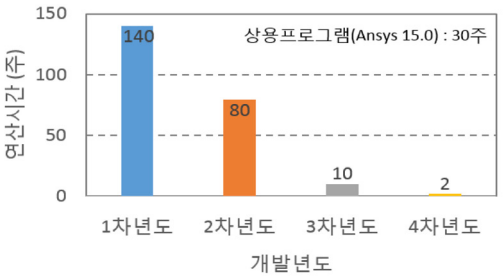


1차년도 : Fixed 기법

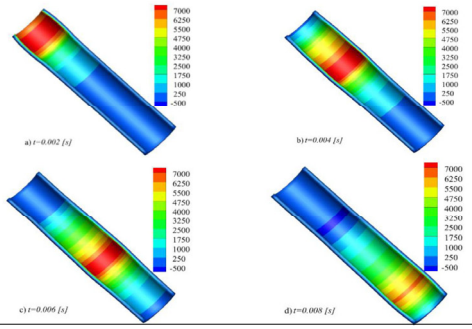
2차년도 : 메모리 최적화

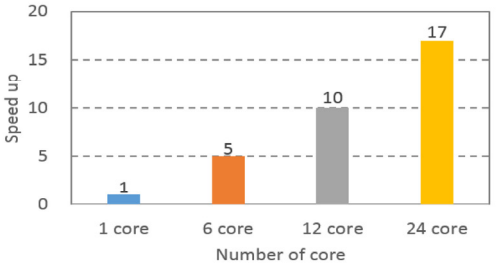
3차년도 : Aitken 기법

4차년도 : 'QN-ILS 기법'



- 단순 혈관 문제에 대한 병렬 알고리즘의 성능 결과



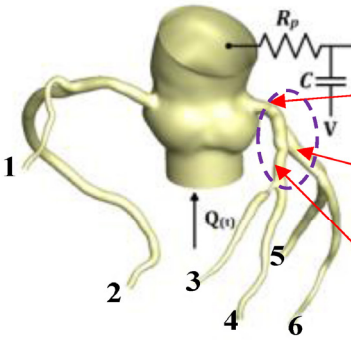


Parallelization

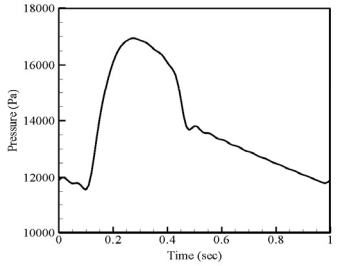
Simulation of clinical trials

- 다양한 임상 환자에 대한 유체-구조 상호작용 문제의 경계조건 획득 방법

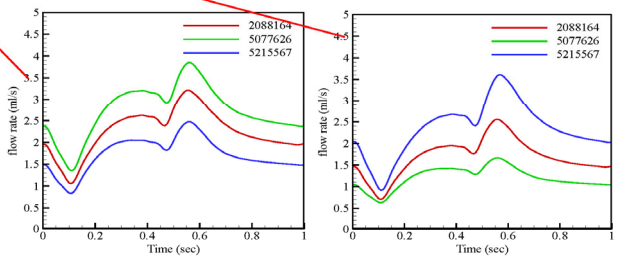
협착이 존재하는 영역 근처만 유체-구조 상호작용 해석 수행



관상동맥 유동 해석 수행
(울산대학교 이상욱교수팀)



압력 데이터 획득

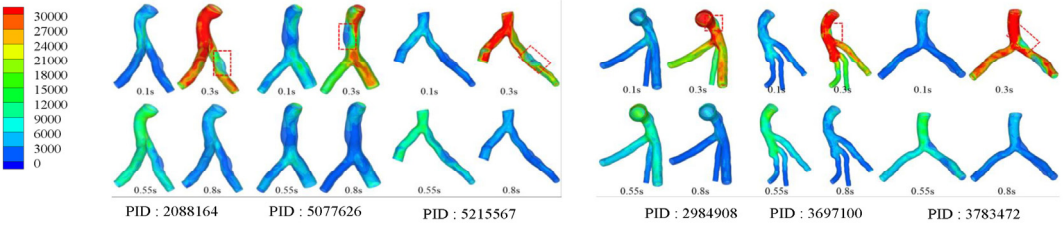


유량 데이터 획득

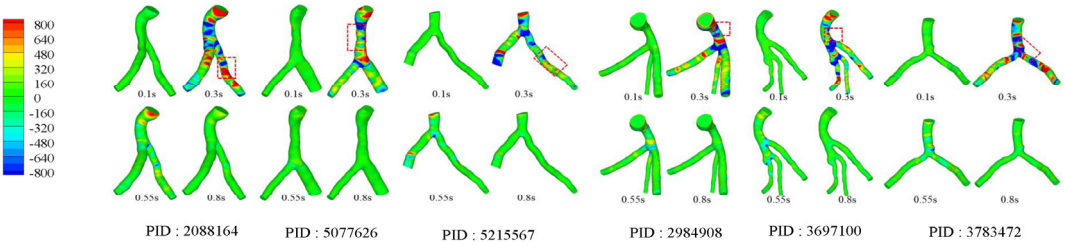
Simulation of clinical trials

- 다양한 임상 환자에 대한 유체-구조 상호작용 해석 (협착 성장에 대한 예후 예측 : 6개월)

Von-mises stress



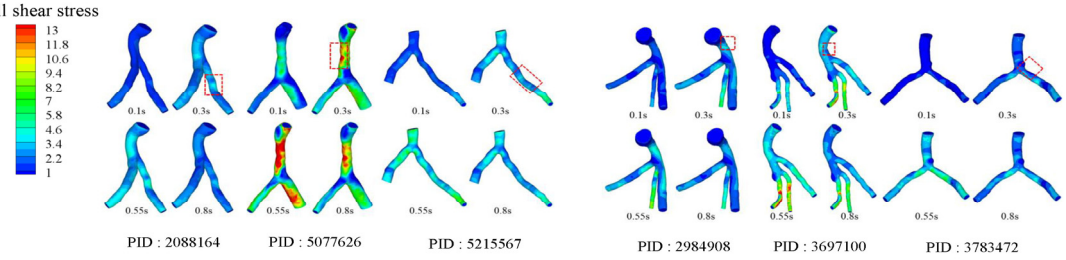
APS(Axial Plaque Stress)



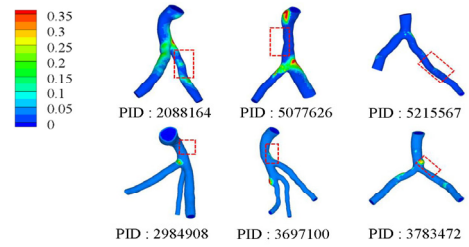
Simulation of clinical trials

- 다양한 임상 환자에 대한 유체-구조 상호작용 해석 (협착 성장에 대한 예후 예측 : 6개월)

Wall shear stress



OSI(Oscillatory shear index)



예측실패

	2088164 (ref.)	5077626	5215567	2984908	3697100	3783472
Von-mises	중	하	하	중	중	중
APS	상	중	중	하	상	상
INS. WSS	하	상	하	하	하	하
OSI	중	하	하	하	중	상

현재 파열 예측 정확도 : 80%
(5명의 환자에 대한 블라인드 테스트)