# Beating heart simulation driven by three dimensional molecular dynamics model

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#### Multiscale Challenge on K-computer (2012)

#### **Model size**

6
6
5
0
0

#### Performance

	Pflop/s			% of peak		
model\#nodes	20736	41472	82944	20736	41472	82944
49KDOF	0.72	1.39	2.74	28.10	27.43	27.72



# $\begin{array}{ll} I\!I\!I\!B & Coronary Circulation \\ \sum_{C(K,J)=C} \overline{\eta}_{K} \left( \overline{\mu}_{C} - \overline{\mu}_{C(K,J)} \right) = 0, \ \forall C \quad \text{(c)} \\ \sum_{c(k,j)=c} \left( \frac{\pi}{4} D_{kj} \dot{D}_{kj} L_{k} + \eta_{k} \left( \mu_{c} - \mu_{c(k,j)} \right) \right) = 0, \ \forall c \ \text{(d)} \\ D_{i}(t) = \beta \cdot \left( (\mu_{i}(t) - \overline{p}_{m}(t)) - (\mu_{i}^{*} - \overline{p}_{m}^{*}) \right) + D_{i}^{*} \ \text{(e)} \\ \Delta V_{cap} = \overline{\omega} \frac{\pi}{8} \sum_{k} L_{k} \sum_{c,j}^{2} \left( D_{kj}^{2} - D_{kj}^{0} \right)^{2} \quad \text{(f)} \end{array}$

#### IIA Macroscopic Muscle and Blood

## **Conventional Multiscale Approach**

#### Heart –Sarcomere Coupling Model



### Research directions for Post-K : from 1d MC to 3d MD





#### Cafemol (Takada Lab., Kyoto Univ.) Focusing on inside of the molecular motor

Switch the potentials at the state transitions



Thin filament (modeled by a rigid bar)

#### Preliminary test using Cafemol-Ring Coupling model



#### Micro-Macro interaction through the thin filament sliding



#### Behavior of the molecular motor under physiological condition



#### **Verification of Pocket Deformation Feedback Model**

Contour of the pocket deformation of the basic model



#### **Verification of Pocket Deformation Feedback Model**

Benefits of the feedback mechanism

- 1. 3% increase of blood ejection
- 2. 10% reduction of ATP consumption



## **Coupling technique : Efficiency & Stability**

- 1. Reduction of communication overheads by the multiple time step method
- 2. Stability by taking the active stiffness



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- Reduction of communication overheads by the multiple time step method 1.
- 2. Stability by taking the active stiffness

Strain in the fiber direction



## **Concluding Remarks**

We constructed a multiscale platform that enables us to analyze the stochastic dynamics of motor proteins under the condition : that is generated by the protein motors themselves that can't be made from artificial boundary conditions

# **Big data & Al**

- Huge numerical simulation data of the molecular behavior
- Seeking correlations between the functional parts in the protein motors
- Optimization of parameters of numerical models

