Calculation method of coefficients of bending energy and non-uniqueness of local stress field

1. **Non-uniqueness of local stress field**

2. **Virtual bending method to calculate coefficients of bending energy**

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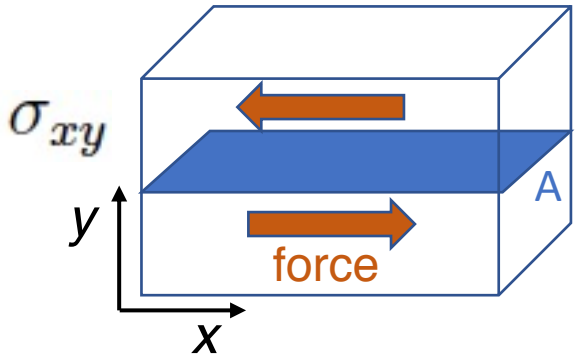
Calculation of global stress in molecular simulation

Stress: force per area



area average

Kinetic component:

Momentum transport via molecular motion

$$\sigma_{xy}^{\mathrm{K}} = \frac{m}{A\Delta t}\Big\langle \sum_{y_i(t)>0, v_{i,y}<-\frac{y_i(t)}{\Delta t}} v_{i,x} - \sum_{y_i(t)<0, v_{i,y}>-\frac{y_i(t)}{\Delta t}} v_{i,x} \Big\rangle$$

up-to-down down-to-up

Potential component:

forces crossing the surface

$$\sigma_{xy}^{\mathrm{U}} = \frac{1}{A}\Big\langle \sum_{y_i>0, y_j<0} f_{i,x}(\mathbf{r}_i, \mathbf{r}_j, \ldots, \mathbf{r}_k) \Big\rangle$$

averaging surfaces

volume average

Virial theorem:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\mathrm{K}} + \boldsymbol{\sigma}_{\mathrm{U}},$$

$$\boldsymbol{\sigma}_{\mathrm{K}} = -\frac{1}{V}\sum_i \langle m_i \mathbf{v}_i \otimes \mathbf{v}_i \rangle,$$

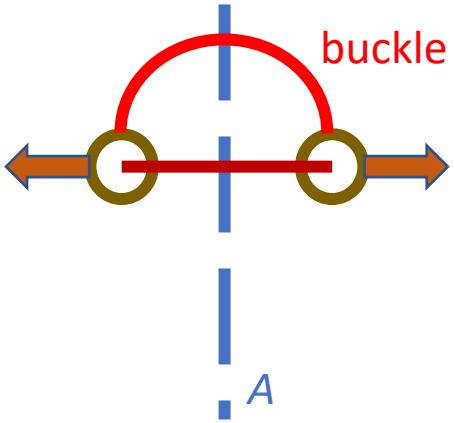
$$\boldsymbol{\sigma}_{\mathrm{U}} = -\frac{1}{V}\sum_i \langle \mathbf{f}_i \otimes \mathbf{r}_i \rangle,$$

Pressure tensor

$$P_{\alpha\beta} = -\sigma_{\alpha\beta}$$

Clear definition. Stress is uniquely determined.

Local stress for pairwise potentials



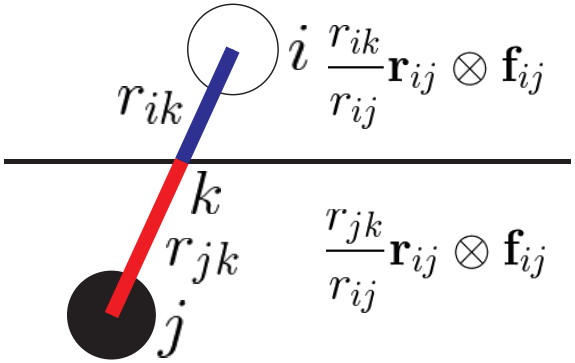
Force propagating through the surface, but lateral position can be different.

Propagating pathway is not uniquely determined.

but

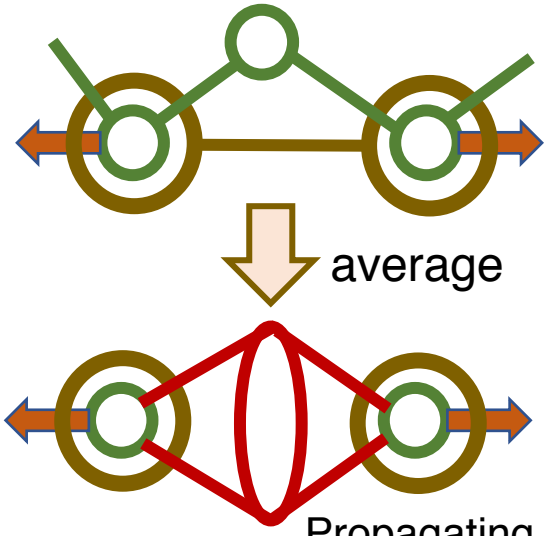
Let's use the straight line for simplicity!

Irving-Kirkwood-Noll (IKN) procedure



Minimizing sum of length, etc.

Coarse-graining from ○ to ○



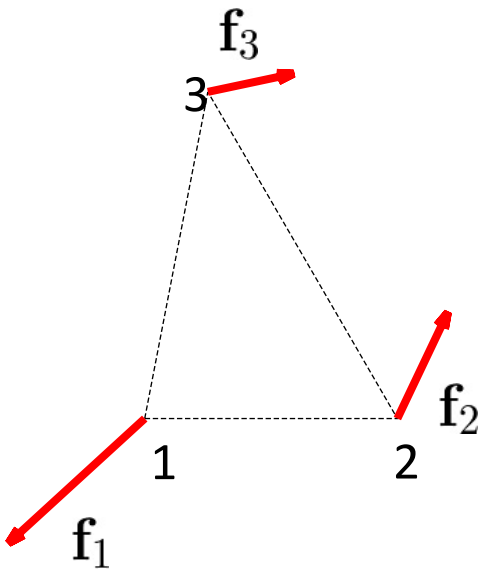
Propagating along cones?

Admal and Tadmor, J. Elast. 100, 63-143 (2010).

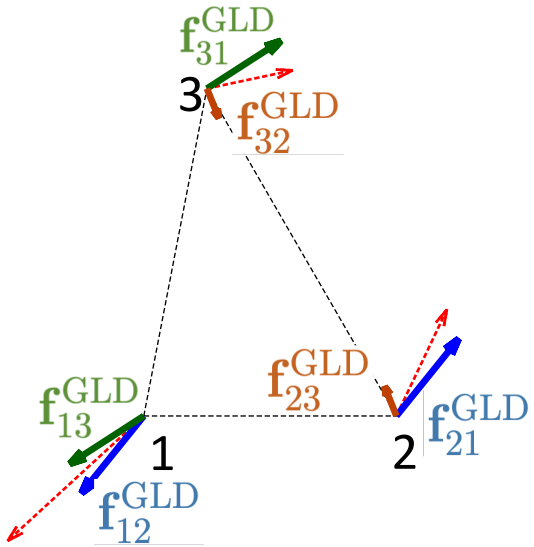
Local stress for multi-body potentials

decomposition to pairwise forces

three-body forces

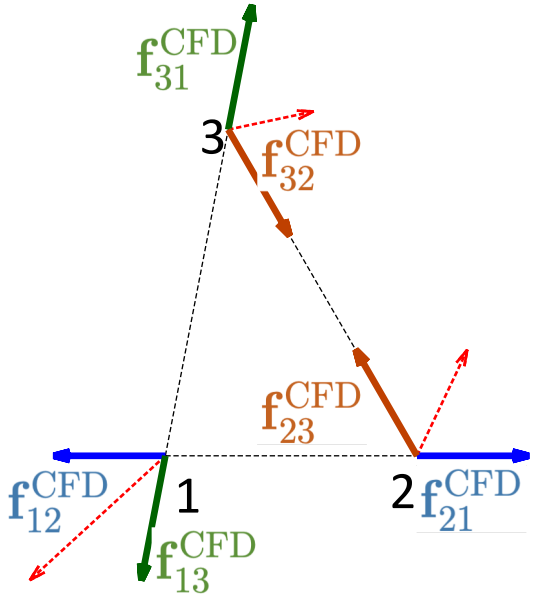


Goetz Lipowsky Decomposition



$$\mathbf{f}_{ij}^{GLD} = (\mathbf{f}_i - \mathbf{f}_j)/n$$

Central Force Decomposition (CFD)

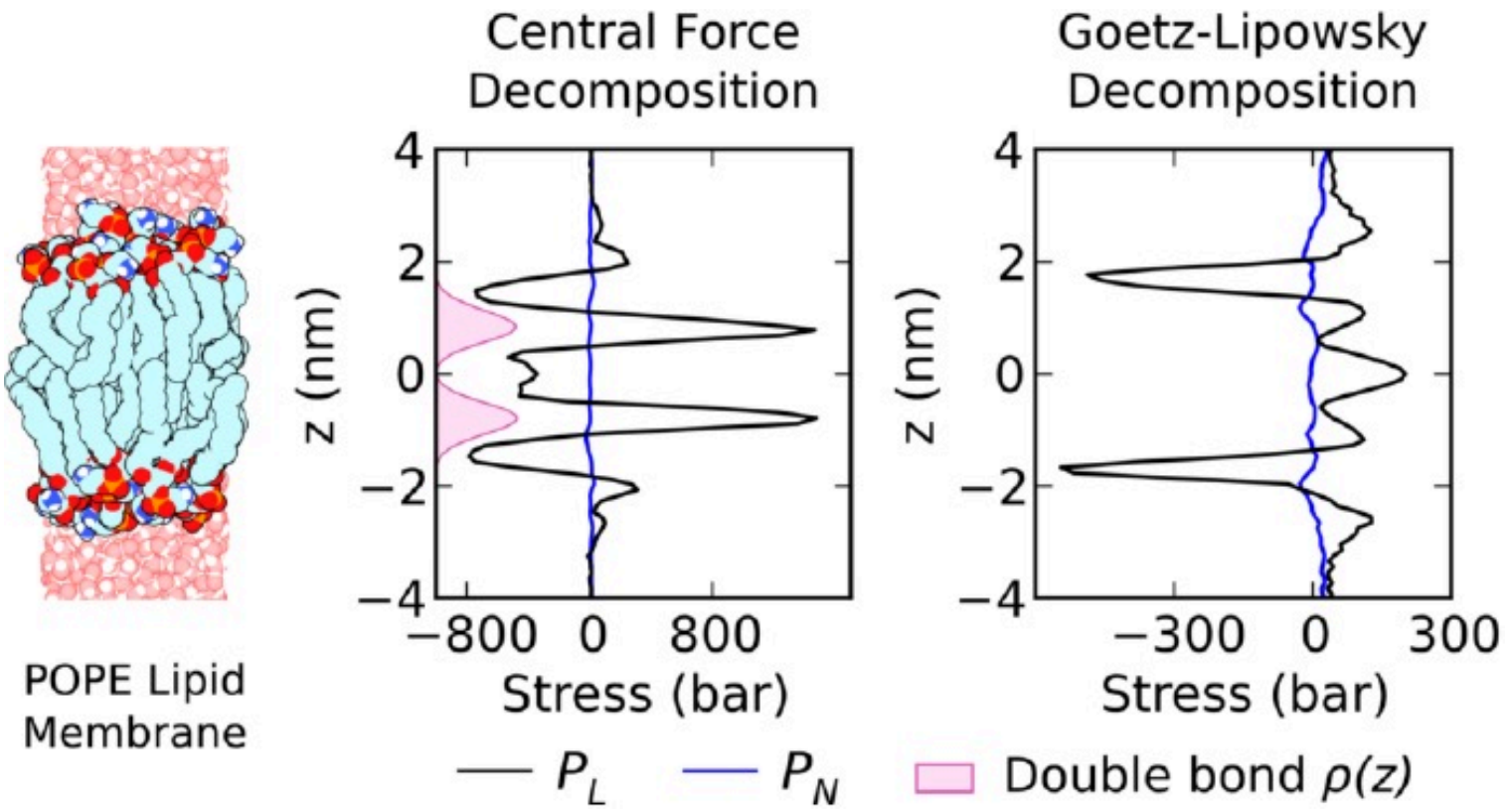


$$\mathbf{f}_{ij}^{CFD} = f_{ij}\hat{\mathbf{r}}_{ij}$$

$\mathbf{r}_{ij} \nparallel \mathbf{f}_{ij}$	$\mathbf{r}_{ij} \parallel \mathbf{f}_{ij}$
$\sigma_{\alpha\beta} \neq \sigma_{\beta\alpha}$	$\sigma_{\alpha\beta} = \sigma_{\beta\alpha}$
Angular momentum not conserved	conserved

Goetz and Lipowsky, J. Chem. Phys. 108, 7397 (1998). Admal and Tadmor, J. Elast. (2010).

Pressure profile of membrane (P=- σ)



Stress profile strongly depends on force decomposition!

Vanegas, Torres-Sànchez, and **Arroyo**, J. Chem. Theory Comput. 10, 691 (2014).

Central Force Decomposition (CFD) for *n*-body potentials

CFD is not unique at n>4 in 3D (n>3 in 2D).

More degrees of freedom
n(n-1)/2 > 3n - 6 in 3D
2n - 3 in 2D

For large *n*, CFD force pairs are give by

$$\boldsymbol{\Psi} = (f_{12}, \ldots, f_{ij}, \ldots)$$

$$\boldsymbol{\Psi} = \boldsymbol{\Psi}_0 + \sum_{\ell}^{n_{\text{rest}}} a_\ell \boldsymbol{\Psi}_\ell$$

$$\boldsymbol{\Psi}_0 \cdot \boldsymbol{\Psi}_\ell = 0$$

a_ℓ is an arbitrary real number.

$\boldsymbol{\Psi}_0$ is called covariant or irrotational component.

(Arroyo) (Admal)

Admal and Tadmor, J. Mech. Phys. Solids 93, 72 (2016).

Torres-Sánchez, Vanegas, and Arroyo, J. Mech. Phys. Solids 93, 224 (2016).

In covariant CFD, Ψ_0 is used as a unique decomposition.

minimization of $\boldsymbol{\Psi}^2 = \sum_{ij} f_{ij}^2$

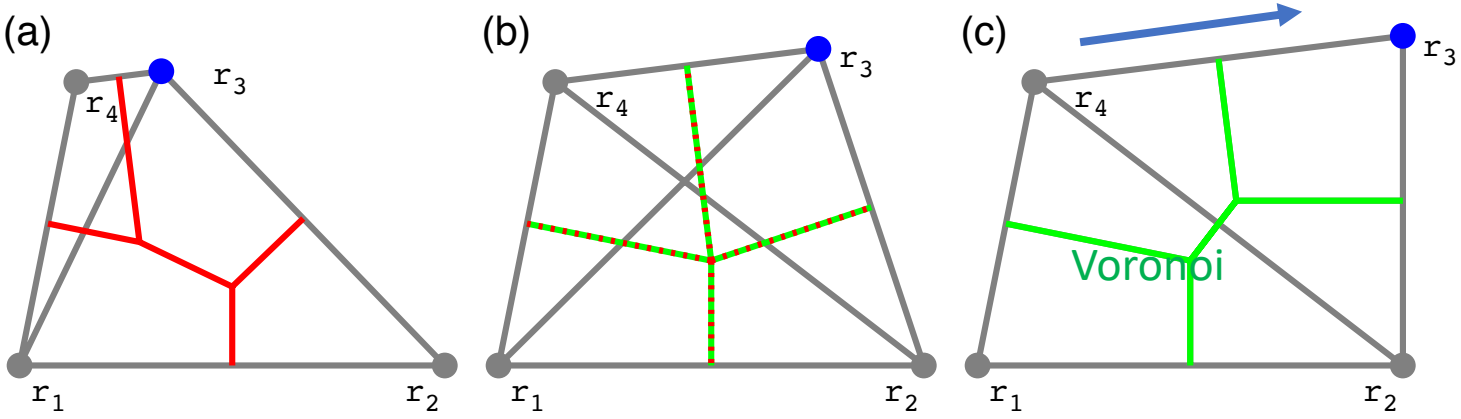
Torres-Sánchez, **Vanegas**, and **Arroyo**, J. Mech. Phys. Solids 93, 224 (2016).

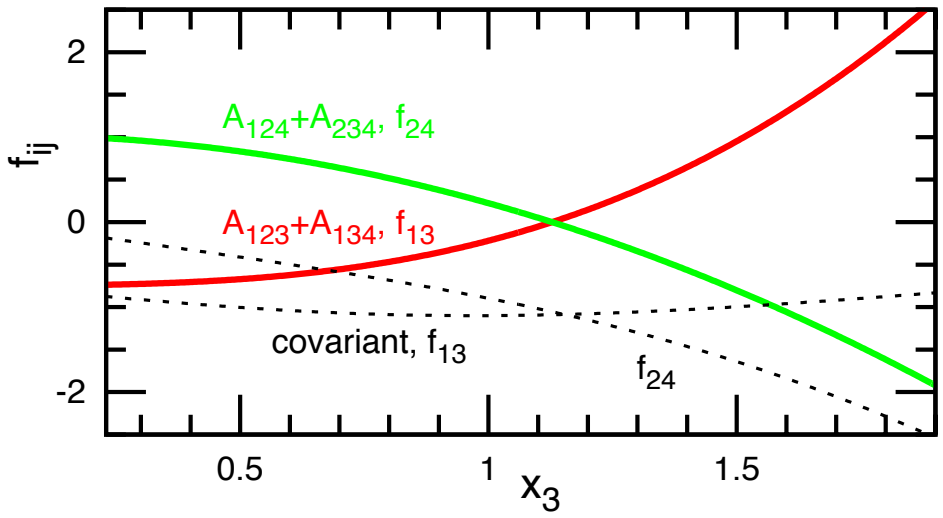
Example of the force decomposition (area of tetragon in 2D)

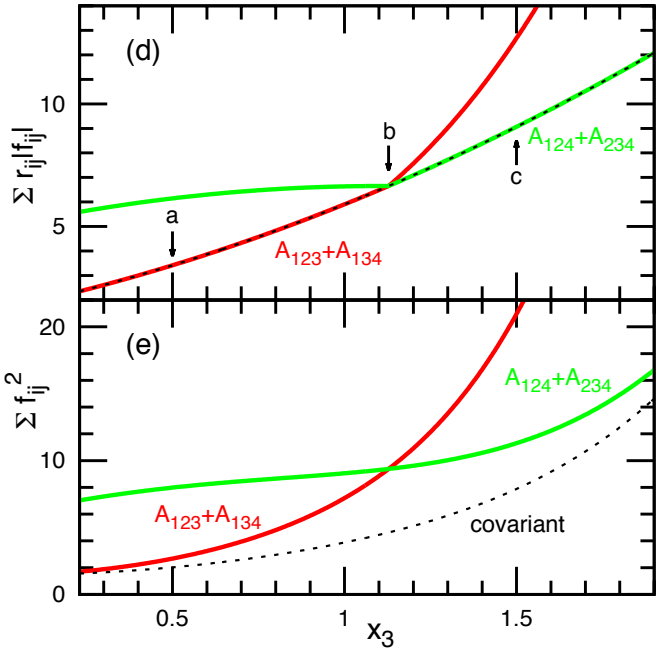
Potential $A_{1234}{}^2$

$$A_{1234} = A_{123} + A_{134} = A_{124} + A_{134}$$

$$\Psi_1 = \Psi(A_{123} + A_{134}) - \Psi(A_{124} + A_{134})$$







Q: Which do you choose, covariant CFD or Voronoi?

Force decomposition of pairwise potentials

Case: a multibody potential expresses a sum of pairwise potentials in some limit.

$$U_{\mathrm{ps}} = \sum_k U_{\mathrm{pair},k}(r_{ij})$$

Force decomposition should be

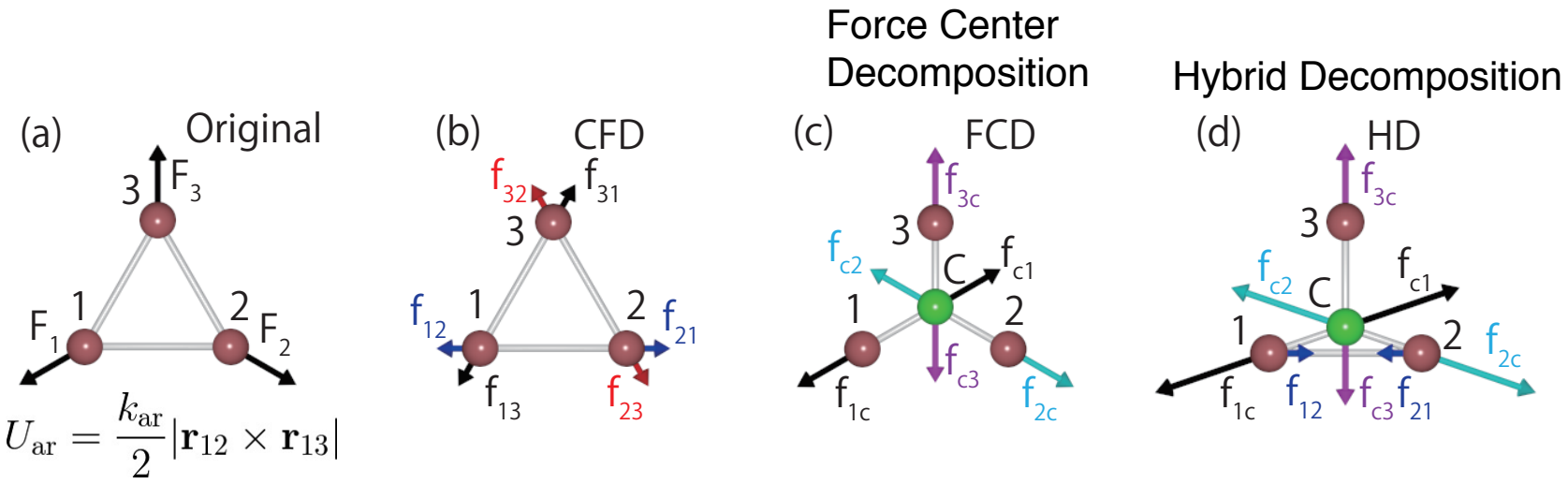
$$f_{ij} = -\frac{\partial U_{\mathrm{pair},k}}{\partial r_{ij}}$$

But

covariant CFD and any other methods only based on f_i cannot give this decomposition.

HN, Phys. Rev. E **102**, 053315 (2020).

Force Center Decomposition (FCD) for three-body potentials



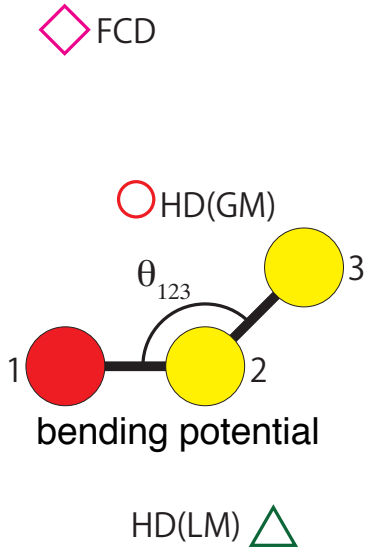
$$U_{\rm ar} = \frac{k_{\rm ar}}{2}|\mathbf{r}_{12} \times \mathbf{r}_{13}|$$

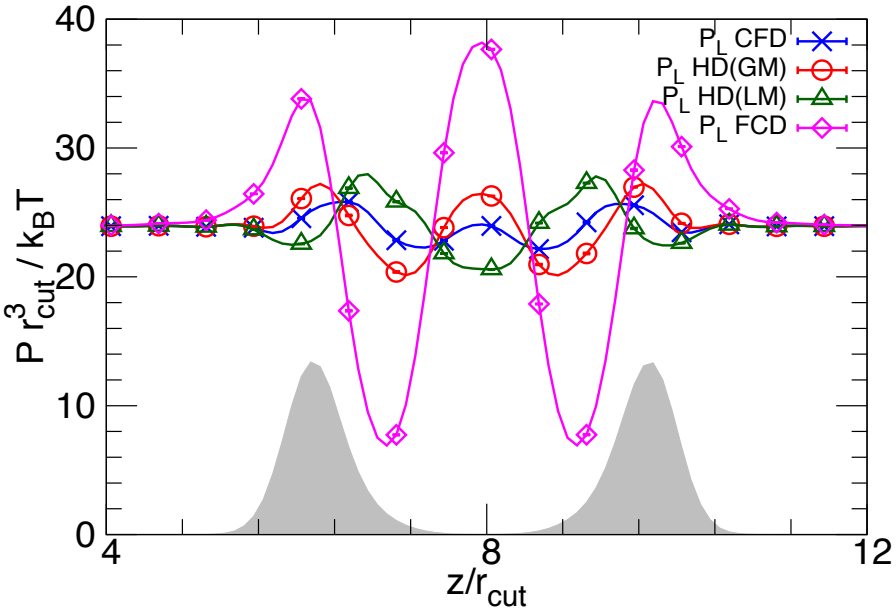
Another decomposition conserving angular momentum

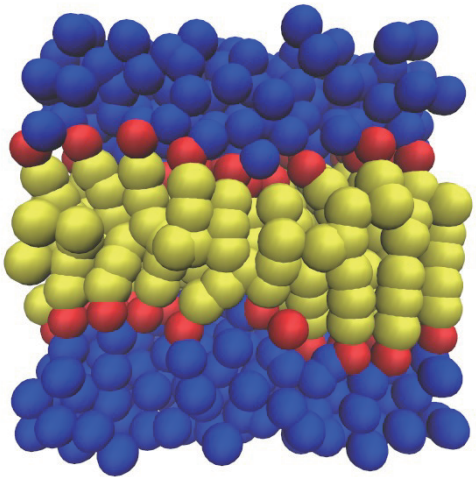
Force Center Decomposition (FCD):
Forces of a three-body potential always meets at one point.
These force pairs can be used for decomposition.

K. M. Nakagawa and HN, Phys. Rev. E **94**, 053304 (2016).

Pressure profile of membrane, again







DPD membrane

Stress profile strongly depends on force decomposition even under the angular-momentum conservation!

But profile is always **mirror-symmetric.**

K. M. Nakagawa and HN, Phys. Rev. E **94**, 053304 (2016).

Summary 1

Local stress filed is not uniquely determined
on molecular scale.

K. M. Nakagawa and HN, Phys. Rev. E **94**, 053304 (2016).
HN, Phys. Rev. E **102**, 053315 (2020).

Questions:

Q1: Is molecular-scale local stress a meaningful quantity?

If yes:

Q2: How do you calculate local stress?

a. From higher resolution data
(quantum calculation for all-atom MD, All-atom for CG)
b. Following some manner (covariant CFD or others)

Q3: Do macroscopic properties depend on the decomposition?

2. Virtual bending method to calculate coefficients of bending energy

Bending energy

$$F = \int \left[\frac{\kappa}{2} (C_1 + C_2 - C_0)^2 + \bar{\kappa} C_1 C_2 \right] dA$$

- Bending rigidity κ
- Saddle-splay modulus (Gaussian modulus) $\bar{\kappa}$
- Spontaneous curvature C_0

Estimation of saddle-splay modulus from stress profile

moments of stress profile

first moment

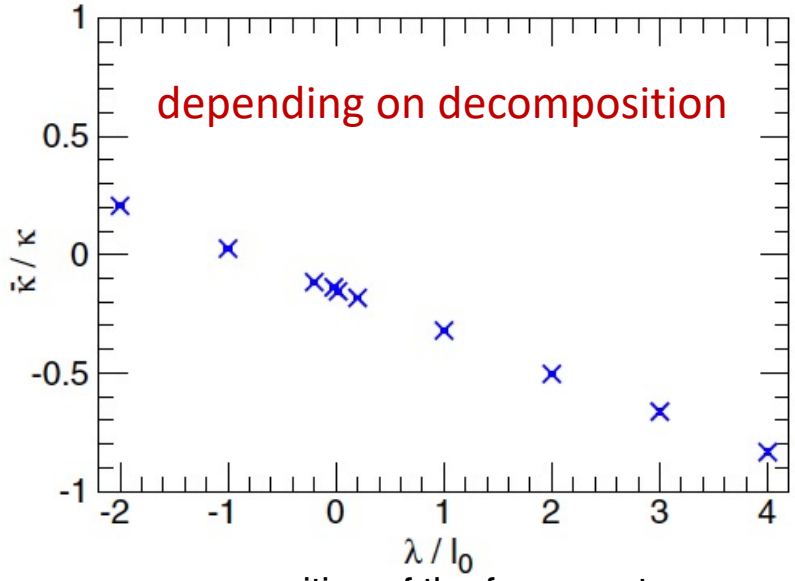
$$-\kappa C_0 = \int (\sigma_{\parallel}(z) - \sigma_{zz}(z)) z \, dz,$$

second moment

$$\bar{\kappa} = \int (\sigma_{\parallel}(z) - \sigma_{zz}(z)) z^2 \, dz,$$

lateral vertical

W. Helfrich, Physics of Defects (1981).
I. Szleifer, D. Kramer, A. Ben-Shaul, W. M. Gelbart, and S. A. Safran, J. Chem. Phys. 92, 6800 (2016).



position of the force center

K. M. Nakagawa and HN, Phys. Rev. E **94**, 053304 (2016).

Q: What's wrong?

?

$$\bar{\kappa}/\kappa \simeq -1$$

for lipid membrane

Hu, Briguglio, and Deserno, Biophys. J. 102, 1403 (2012).

Aim:

Calculating $\kappa, \bar{\kappa}, C_0$

directly from mechanical response

without using force decomposition

Free energy change by virtual deformation (parameter λ)

$$F = -k_{\mathrm{B}}T \ln\left(\int e^{-E/k_{\mathrm{B}}T}\, d\Omega\right),$$

$$\left.\frac{\partial F}{\partial \lambda}\right|_{V,T} = \frac{\int \frac{\partial E}{\partial \lambda} e^{-E/k_{\mathrm{B}}T} d\Omega}{\int e^{-E/k_{\mathrm{B}}T} d\Omega} = \left\langle \frac{\partial E}{\partial \lambda} \right\rangle_{V,T},$$

$$\left.\frac{\partial^2 F}{\partial \lambda^2}\right|_{V,T} = \left\langle \frac{\partial^2 E}{\partial \lambda^2} \right\rangle_{V,T} - \frac{1}{k_{\mathrm{B}}T}\left(\left\langle \left(\frac{\partial E}{\partial \lambda}\right)^2 \right\rangle_{V,T} - \left\langle \frac{\partial E}{\partial \lambda} \right\rangle_{V,T}^2\right),$$

thermal-fluctuation term

This is not considered in stress profile method.

A: Second moment ≠ $\bar{\kappa}$

Example of virtual deformation (calculation of surface tension γ)

affine deformation (constant volume, lateral extension)

$$\mathbf{r}_i' = \begin{pmatrix} 1+\varepsilon/2 & 0 & 0 \\ 0 & 1+\varepsilon/2 & 0 \\ 0 & 0 & 1-\varepsilon \end{pmatrix} \mathbf{r}_i$$

virtual work

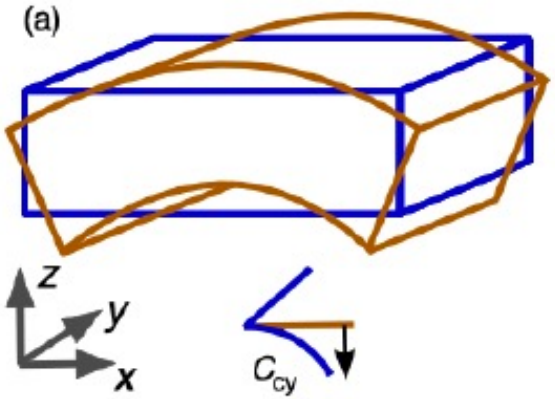
$$\Delta F = \gamma \Delta A_{xy} \qquad \Delta A_{xy} = \varepsilon A_{xy}$$

$$\gamma = \frac{1}{A_{xy}} \sum_i \left\langle \frac{1}{2}\left(x_i \frac{\partial U}{\partial x_i} + y_i \frac{\partial U}{\partial y_i} \right) - z_i \frac{\partial U}{\partial z_i} \right\rangle$$
$$= [(\sigma_{xx} + \sigma_{yy})/2 - \sigma_{zz}]/A_{xy}$$

same form as in usual method of stress difference

Virtual bending deformation

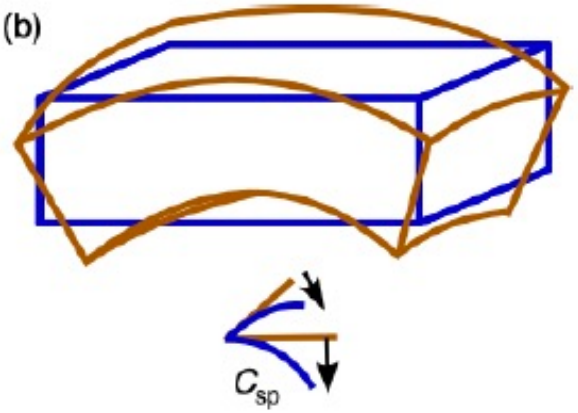
Cylindrical deformation



$$F = \frac{\kappa}{2}(C_{\mathrm{cy}} - C_0)^2 A_{xy}$$

κ and C_0

Spherical deformation



$$F = \left[\frac{\kappa}{2}(2C_{\mathrm{sp}} - C_0)^2 + \bar{\kappa} C_{\mathrm{sp}}^2\right] A_{xy}$$

also, $\bar{\kappa}$

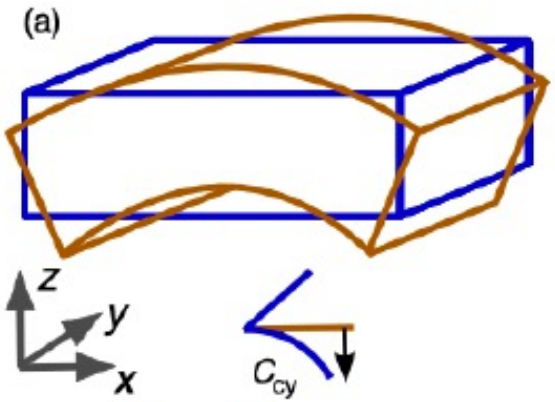
Local deformation with constant curvature is available under periodic boundary condition.
(not for longer-range interactions than length of simulation box)

$$\left.\frac{\partial F}{\partial C_{\mathrm{cy}}}\right|_{V,T,C_{\mathrm{cy}}=0} = -\kappa C_0 A_{xy} = \left\langle \frac{\partial U}{\partial C_{\mathrm{cy}}} \right\rangle, \tag{16}$$

$$\left.\frac{\partial^2 F}{\partial C_{\mathrm{cy}}^2}\right|_{V,T,C_{\mathrm{cy}}=0} = \kappa A_{xy} = \left\langle \frac{\partial^2 U}{\partial C_{\mathrm{cy}}^2} \right\rangle - \frac{1}{k_{\mathrm{B}}T}\left(\left\langle \left(\frac{\partial U}{\partial C_{\mathrm{cy}}}\right)^2 \right\rangle - \left\langle \frac{\partial U}{\partial C_{\mathrm{cy}}} \right\rangle^2\right), \tag{17}$$

$$\left.\frac{\partial^2 F}{\partial C_{\mathrm{sp}}^2}\right|_{V,T,C_{\mathrm{sp}}=0} = (4\kappa + 2\bar{\kappa}) A_{xy} = \left\langle \frac{\partial^2 U}{\partial C_{\mathrm{sp}}^2} \right\rangle - \frac{1}{k_{\mathrm{B}}T}\left(\left\langle \left(\frac{\partial U}{\partial C_{\mathrm{sp}}}\right)^2 \right\rangle - \left\langle \frac{\partial U}{\partial C_{\mathrm{sp}}} \right\rangle^2\right), \tag{18}$$

Cylindrical deformation



$$U(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{n=2}^{N} \sum_{k_n} U_{k_n}(\mathbf{r}_{k_n,1}, ..., \mathbf{r}_{k_n,n}),$$

$$\delta U_{k_n} \simeq \sum_{j}^{n} \left(\delta x_j \frac{\partial U_{k_n}}{\partial x_j} + \delta y_j \frac{\partial U_{k_n}}{\partial y_j} + \delta z_j \frac{\partial U_{k_n}}{\partial z_j} \right) \quad (26)$$

$$+ \frac{1}{2} \left(\sum_{j}^{n} \delta x_j \frac{\partial}{\partial x_j} + \delta y_j \frac{\partial}{\partial y_j} + \delta z_j \frac{\partial}{\partial z_j} \right)^2 U_{k_n}.$$

$$\theta_{c,i} = C_{cy} x_i,$$

$$r'_{c,i} = \frac{1}{C_{cy}} + z_i - \frac{1}{2} z_i^2 C_{cy} + \frac{\alpha_1}{2} z_i^3 C_{cy}^2.$$

constant volume: $\alpha_1 = 1$

variable α_1 to check volume fluctuation effects

$$x'_i = r'_i \sin\theta_{c,i},$$

$$y'_i = y_i,$$

$$z'_i = r'_i \cos\theta_{c,i} - \frac{1}{C_{cy}},$$

$$x'_i = x_i \left[1 + z_i C_{cy} - \left(\frac{z_i^2}{2} + \frac{x_i^2}{6} \right) C_{cy}^2 \right] + O(C_{cy}^3),$$

$$z'_i = z_i - \frac{1}{2}(z_i^2 + x_i^2) C_{cy} + \frac{z_i}{2}(\alpha_1 z_i^2 - x_i^2) C_{cy}^2 + O(C_{cy}^3).$$

$$\left\langle \frac{\partial U_{k_n}}{\partial C_{cy}} \right\rangle = \sum_{j}^{n} \left\langle \frac{z_j}{2} \left(x_j \frac{\partial U_{k_n}}{\partial x_j} + y_j \frac{\partial U_{k_n}}{\partial y_j} \right) \right. \quad (27)$$

$$\left. - \left(\frac{z_j^2}{2} + \frac{x_j^2 + y_j^2}{4} \right) \frac{\partial U_{k_n}}{\partial z_j} \right\rangle,$$

$$\left\langle \frac{\partial^2 U_{k_n}}{\partial C_{cy}^2} \right\rangle = \sum_{j}^{n} \left\langle - x_j \left(\frac{z_j^2}{2} + \frac{x_j^2}{6} \right) \frac{\partial U_{k_n}}{\partial x_j} \right. \quad (28)$$

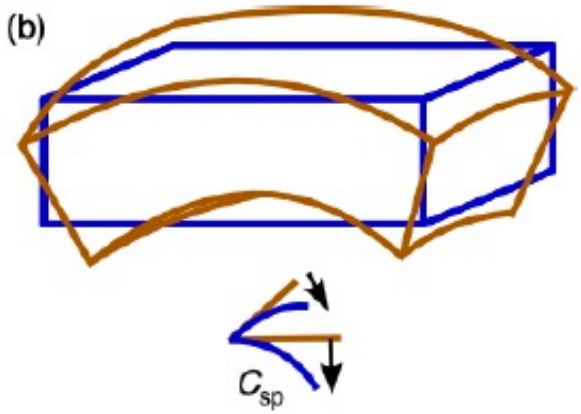
$$- y_j \left(\frac{z_j^2}{2} + \frac{y_j^2}{6} \right) \frac{\partial U_{k_n}}{\partial y_j}$$

$$\left. + z_j \left(\alpha_1 z_j^2 - \frac{x_j^2 + y_j^2}{2} \right) \frac{\partial U_{k_n}}{\partial z_j} \right\rangle$$

$$+ \frac{1}{2} \left\langle \left(\sum_{j}^{n} x_j z_j \frac{\partial}{\partial x_j} - \frac{z_j^2 + x_j^2}{2} \frac{\partial}{\partial z_j} \right)^2 U_{k_n} \right.$$

$$\left. + \left(\sum_{j}^{n} y_j z_j \frac{\partial}{\partial y_j} - \frac{z_j^2 + y_j^2}{2} \frac{\partial}{\partial z_j} \right)^2 U_{k_n} \right\rangle.$$

Spherical deformation



$$\rho_i = \sqrt{x_i^2 + y_i^2}$$

$$\rho_i' = r_{s,i}' \sin\theta_{s,i} \tag{23}$$
$$= \rho_i \left[1 + z_i C_{sp} - \left(z_i^2 + \frac{\rho_i^2}{6}\right) C_{sp}^2\right] + O(C_{sp}^3),$$

$$z_i' = r_{s,i}' \cos\theta_{s,i} - \frac{1}{C_{sp}} \tag{24}$$
$$= z_i - \left(z_i^2 + \frac{\rho_i^2}{2}\right) C_{sp} + z_i \left(\frac{5\alpha_2}{3} z_i^2 - \frac{\rho_i^2}{2}\right) C_{sp}^2 + O(C_{sp}^3).$$

constant volume: $\alpha_2 = 1$

$$\left\langle \frac{\partial^2 U_{k_n}}{\partial C_{sp}^2} \right\rangle = \sum_j^n \left\langle -\left(2z_j^2 + \frac{x_j^2 + y_j^2}{3}\right)\left(x_j \frac{\partial U_{k_n}}{\partial x_j} + y_j \frac{\partial U_{k_n}}{\partial y_j}\right) \right.$$
$$\left. + z_j \left[\frac{10}{3}\alpha_2 z_j^2 - (x_j^2 + y_j^2)\right] \frac{\partial U_{k_n}}{\partial z_j} \right\rangle$$
$$+ \left\langle \left[\sum_j^n x_j z_j \frac{\partial}{\partial x_j} + y_j z_j \frac{\partial}{\partial y_j}\right.\right.$$
$$\left.\left. - \left(z_j^2 + \frac{x_j^2 + y_j^2}{2}\right) \frac{\partial}{\partial z_j}\right]^2 U_{k_n} \right\rangle. \tag{29}$$

Pairwise potential

$$\left\langle \frac{\partial U_{\text{pair}}}{\partial C_{\text{cy}}} \right\rangle = \left\langle \left(\frac{\rho_{ij}^2}{2} - z_{ij}^2 \right) \frac{z_{\text{G}}}{r_{ij}} \frac{\partial U_{\text{pair}}}{\partial r_{ij}} \right\rangle,$$

$$\left\langle \frac{\partial^2 U_{\text{pair}}}{\partial C_{\text{cy}}^2} \right\rangle = \left\langle \left(\frac{3\alpha_1 + 1}{2} z_{ij}^2 z_{\text{G}}^2 + \frac{\alpha_1}{4} z_{ij}^4 - \frac{x_{ij}^4 + y_{ij}^4}{24} - \frac{\rho_{ij}^2 z_{ij}^2}{4} \right) \frac{1}{r_{ij}} \frac{\partial U_{\text{pair}}}{\partial r_{ij}} + \frac{z_{\text{G}}^2}{2} \left[(x_{ij}^2 - z_{ij}^2)^2 + (y_{ij}^2 - z_{ij}^2)^2 \right] \left(\frac{1}{r_{ij}^2} \frac{\partial^2 U_{\text{pair}}}{\partial r_{ij}^2} - \frac{1}{r_{ij}^3} \frac{\partial U_{\text{pair}}}{\partial r_{ij}} \right) \right\rangle,$$

$$\left\langle \frac{\partial^2 U_{\text{pair}}}{\partial C_{\text{sp}}^2} \right\rangle = \left\langle \left[(10\alpha_2 + 4) z_{ij}^2 z_{\text{G}}^2 - \rho_{ij}^2 z_{\text{G}}^2 - \frac{3\rho_{ij}^2 z_{ij}^2}{4} - \frac{\rho_{ij}^4}{12} + \frac{5\alpha_2 z_{ij}^4}{6} \right] \frac{1}{r_{ij}} \frac{\partial U_{\text{pair}}}{\partial r_{ij}} + \left(\rho_{ij}^4 + 4z_{ij}^4 - 4\rho_{ij}^2 z_{ij}^2 \right) z_{\text{G}}^2 \left(\frac{1}{r_{ij}^2} \frac{\partial^2 U_{\text{pair}}}{\partial r_{ij}^2} - \frac{1}{r_{ij}^3} \frac{\partial U_{\text{pair}}}{\partial r_{ij}} \right) \right\rangle, \quad (32)$$

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$$

$$\mathbf{r}_{\text{G}} = (\mathbf{r}_i + \mathbf{r}_j)/2$$

Relation between first derivative and first stress moment

$$-\kappa C_0 A_{xy} = \left\langle \frac{\partial U}{\partial C_{\mathrm{cy}}} \right\rangle$$

$$\frac{\partial U_{k_n}}{\partial C_{\mathrm{cy}}} = \sum_j^n \frac{z_j}{2}\left(x_j \frac{\partial U_{k_n}}{\partial x_j} + y_j \frac{\partial U_{k_n}}{\partial y_j}\right) - \left(\frac{z_j^2}{2} + \frac{x_j^2 + y_j^2}{4}\right)\frac{\partial U_{k_n}}{\partial z_j}$$

$$= -\sum \left(\frac{\rho_{ij}^2}{2} - z_{ij}^2\right)\frac{z_{\mathrm{G}}}{r_{ij}} f_{ij}$$ = stress moment of central force decomposition

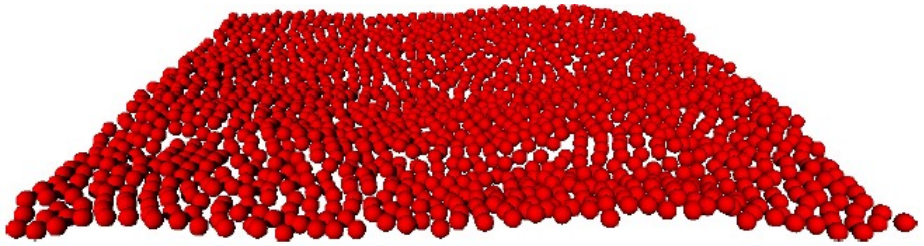
The first derivative coincides with first stress moment, so that it is the discretization form of stress moment without using force decomposition.

FCD gives the same moment, whereas GLD does not.
Angular-momentum-conservation is required for obtaining the right fist moment.

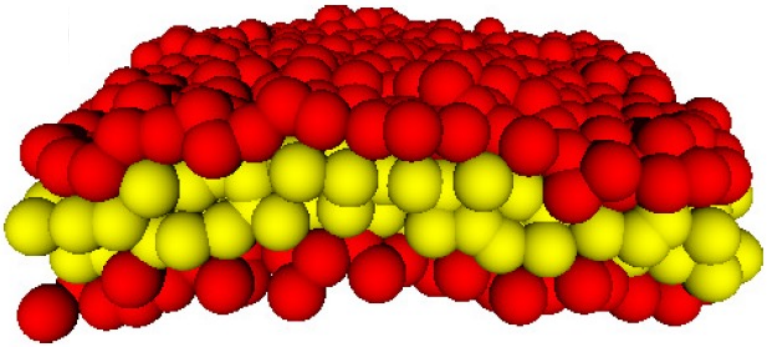
Slide 10: mirror-symmetry -> $C_0 = 0$

Calculation of $\kappa, \bar{\kappa}$ by virtual bending method

1. meshless membrane model
   no solvent
   n-body potential
   $n \sim 20$

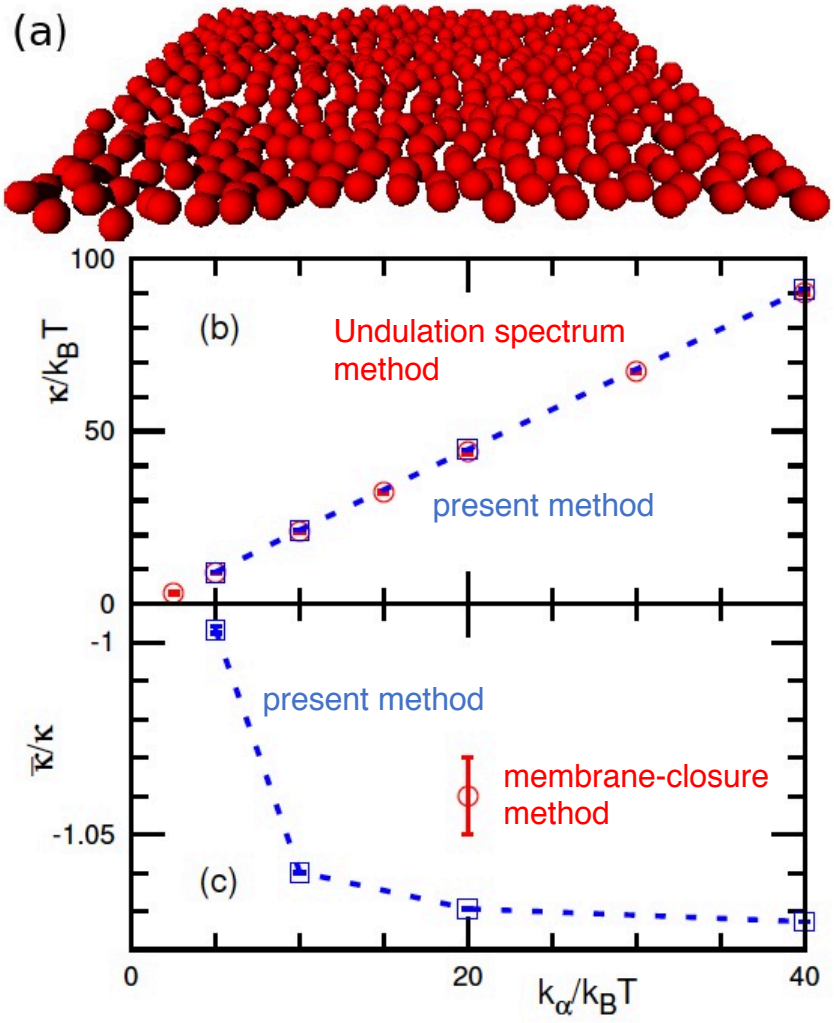


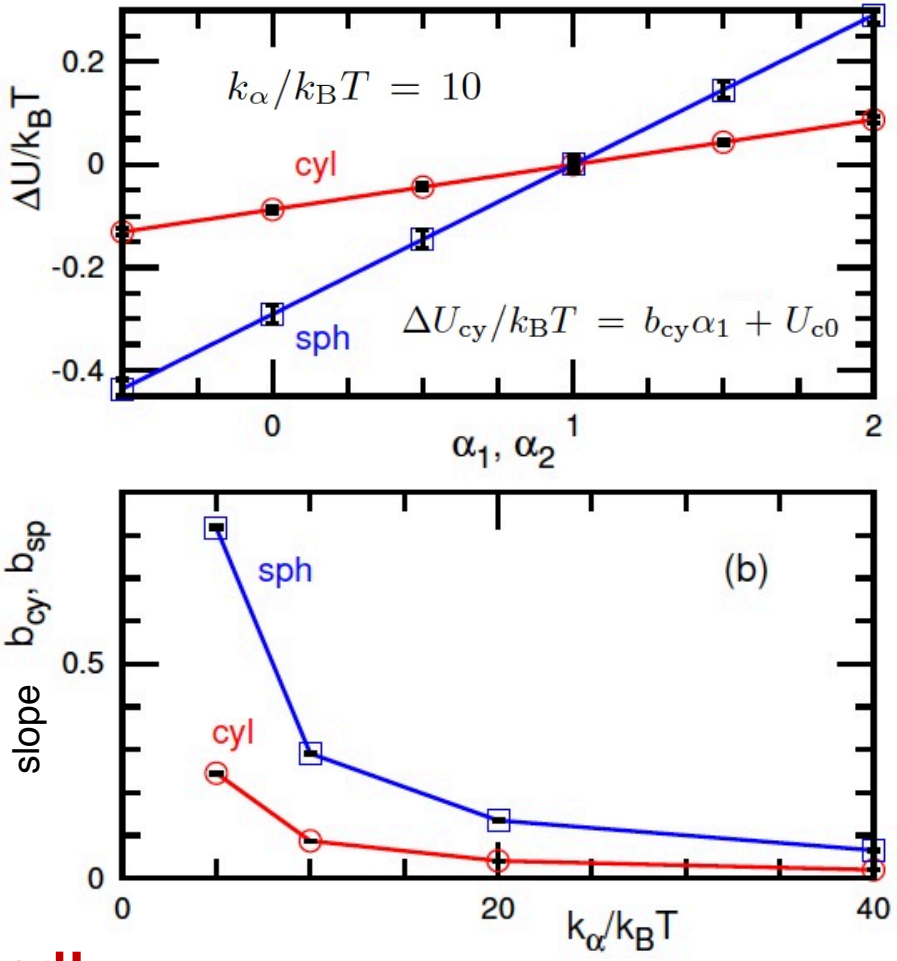
2. DPD membrane model
   with explicit solvent
   two-particle amphiphiles



1. meshless membrane

$$U = k_\alpha \sum_i \alpha_{\rm pl}(\mathbf{r}_i) + \varepsilon\{\sum_{i<j} U_{\rm rep}(r_{i,j}) + \sum_i U_{\rm att}(\rho_i)\}$$

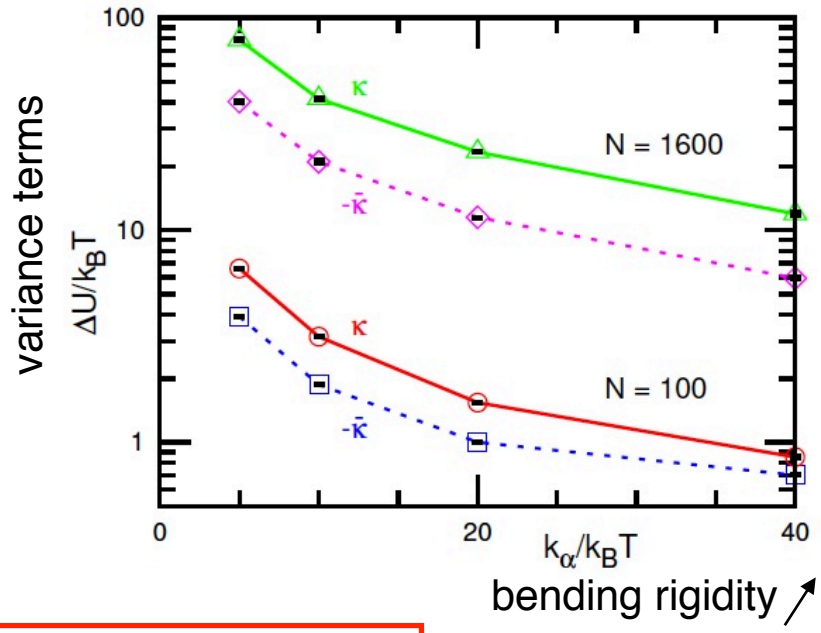




κ, $\bar{\kappa}$ are accurately estimated!

α-dependence (volume-fluctuation effects) is very small.

Influence of membrane fluctuations



$$\left.\frac{\partial^2 F}{\partial C_{\mathrm{cy}}^2}\right|_{V,T,C_{\mathrm{cy}}=0} = \kappa A_{xy} = \left\langle \frac{\partial^2 U}{\partial C_{\mathrm{cy}}^2} \right\rangle - \frac{1}{k_{\mathrm{B}}T}\left(\left\langle \left(\frac{\partial U}{\partial C_{\mathrm{cy}}} \right)^2 \right\rangle - \left\langle \frac{\partial U}{\partial C_{\mathrm{cy}}} \right\rangle^2 \right),$$

$$\left.\frac{\partial^2 F}{\partial C_{\mathrm{sp}}^2}\right|_{V,T,C_{\mathrm{sp}}=0} = (4\kappa + 2\bar{\kappa}) A_{xy} = \left\langle \frac{\partial^2 U}{\partial C_{\mathrm{sp}}^2} \right\rangle - \frac{1}{k_{\mathrm{B}}T}\left(\left\langle \left(\frac{\partial U}{\partial C_{\mathrm{sp}}} \right)^2 \right\rangle - \left\langle \frac{\partial U}{\partial C_{\mathrm{sp}}} \right\rangle^2 \right)$$

Variance terms are larger at larger membrane, but the difference are cancelled with other terms so that values of κ, $\bar{\kappa}$ are unchanged.

Variance terms are far from negligible.

Simple DPD liquid (no membrane, i.e., $\kappa = \bar{\kappa} = 0$)

soft repulsion

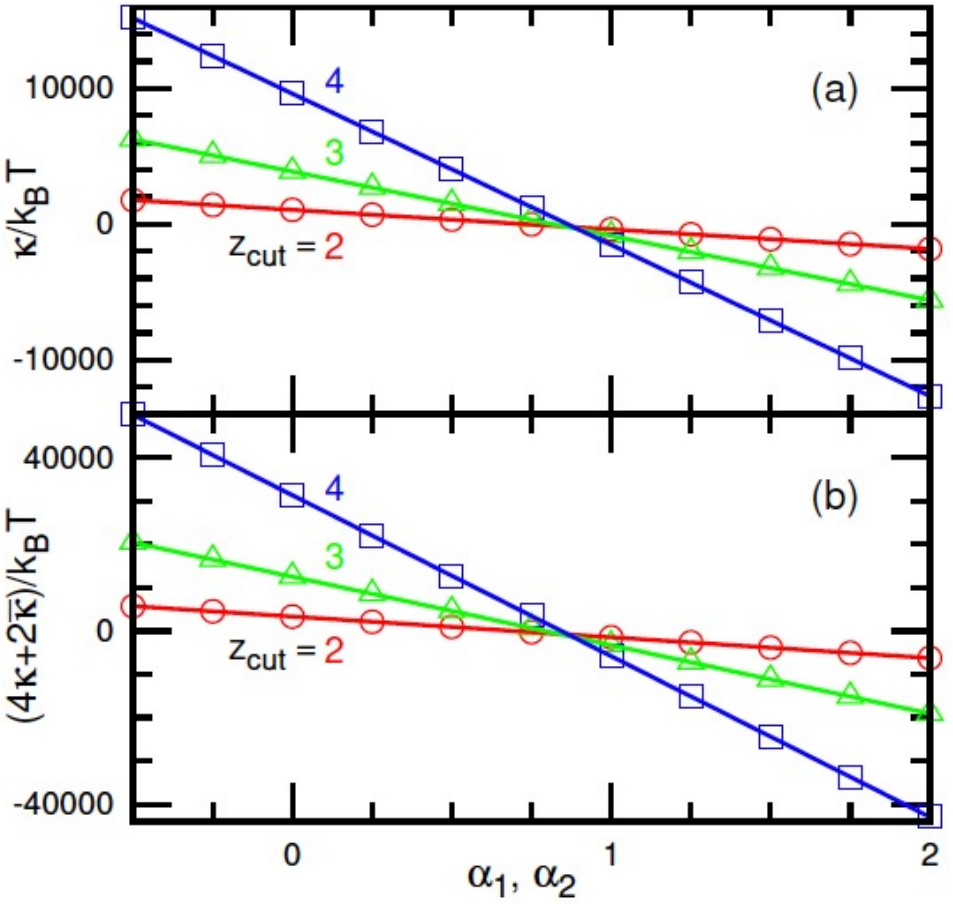
$$U = \sum \frac{a}{2}\left(\frac{r_{ij}}{r_{\rm cut}} - 1\right)^2 \Theta(r_{\rm cut} - r_{ij})$$

$a = 100 k_B T$

calculated for the region

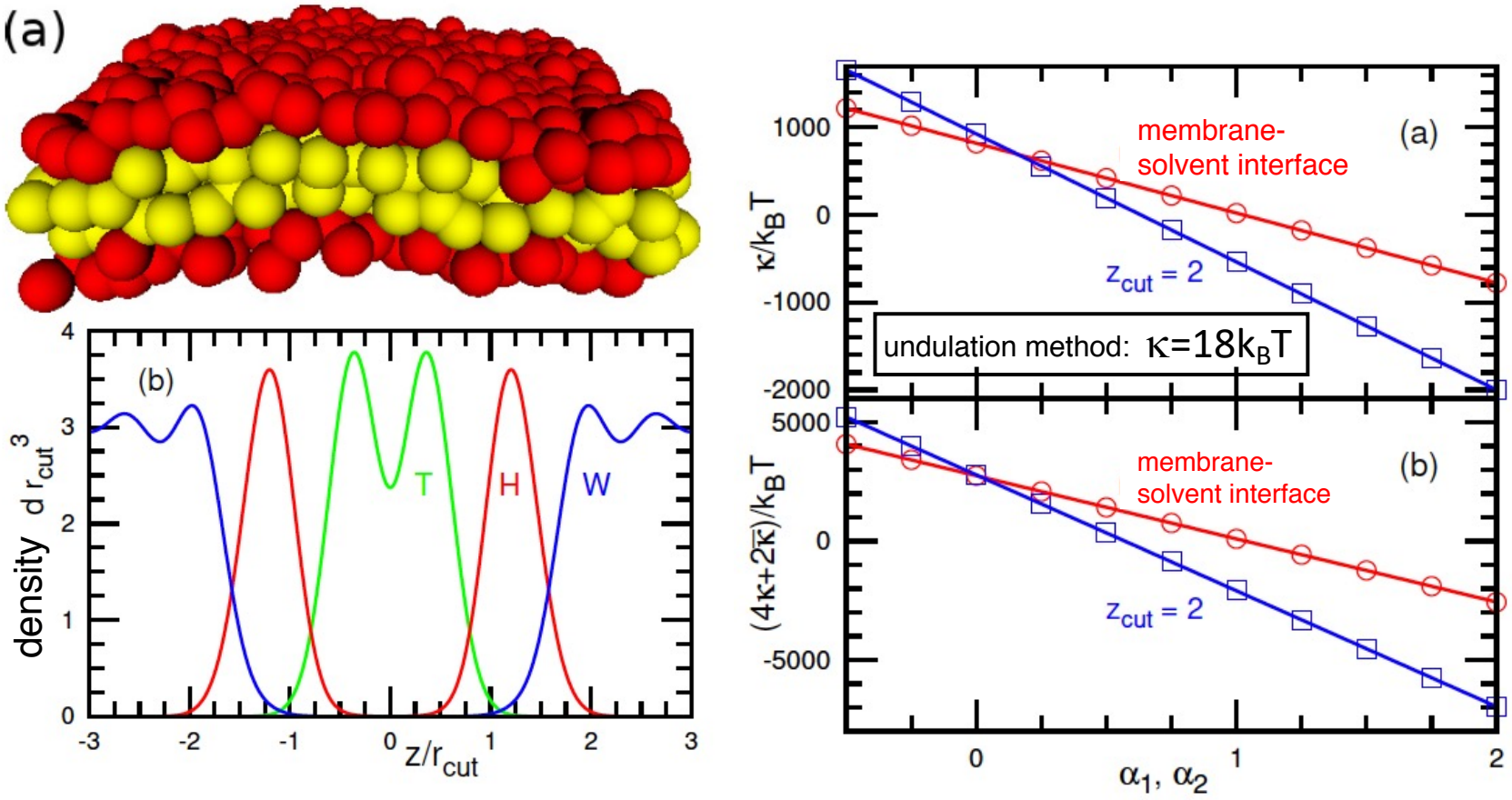
$$|z| < z_{\rm cut}$$

$\kappa = 0$ or $\bar{\kappa} = 0$ is obtained at $\alpha_1, \alpha_2 = 0.7$–0.9.



α-dependence is huge.

2. DPD bilayer membrane



Right values are obtained at $\alpha_1 = \alpha_2 = 1.0$ for cutoff of membrane interface, but α-dependence is terrible.

The method itself looks fine but one more thing is required for accurate estimation.

Summary 2

For meshless membranes, bending rigidity and saddle-splay modulus are accurately calculated by virtual bending method.
For thick membrane with explicit solvent, further extension is required for accurate estimation.

HN, Phys. Rev. E **102**, 053315 (2020).

Questions:

Q3: Do macroscopic properties depend on the decomposition?
First stress moment: ($-\kappa C_0$) independent of decomposition
Second moment: (not $\bar{\kappa}$) dependent on decomposition

Q4: How are the volume fluctuations included in this method?

Q5: Is the virtual deformation method applicable to other deformations such as twisting?

Summary of Questions

Q1: Is molecular-scale local stress a meaningful quantity?

If yes:

Q2: How do you calculate local stress?

a. From higher resolution data
(quantum calculation for all-atom MD, All-atom for CG)

b. Following some manner (covariant CFD or others)

Q3: Do macroscopic properties depend on the decomposition?

Q4: How are the volume fluctuations included in this method?

Q5: Is the virtual deformation method applicable to other deformations such as twisting?

Thank you for your attention &
Looking forward for discussion!

https://noguchi.issp.u-tokyo.ac.jp/rabit_ves.mp4