BOUNDARY CONTROLS AND INTERCONNECTION FOR SCALABLE HAMILTONIAN SYSTEMS GOVERNED BY MOLECULAR DYNAMICS

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Abstract

This paper derives a unified framework of boundary controls and numerical calculus from a scaling free molecular dynamics, called a renormalized molecular dynamics. A renormalized molecular dynamics is suitable not only for the fast numerical calculation of microscopic targets like polymers, but also that of macroscopic targets like mechanical systems because of coarse graining. First, we introduce renormalized Hamiltonian systems. The problem of developing boundary controls in renormalized Hamiltonian systems is that the boundaries of renormalized Hamiltonian systems are not directly derived from molecular dynamics. Thus, we derive the continuum representation of renormalized Hamiltonian systems from the inverse limit of coarse graining. Then, we define a standard boundary control representation of renormalized Hamiltonian systems by using distributed port-Hamiltonian systems. Finally, we will show some numerical examples.

Key words

Hamiltonian systems, Molecular dynamics, Renormalizations, Boundary controls, Distributed parameter systems

1 Introduction

The purpose of this paper is to create a unified framework of boundary controls and numerical calculus from a scaling free molecular dynamics (MD), called renormalized molecular dynamics (RMD). MD method [Thijssen, 1999] is used for reproducing behaviors of microscopic targets. MD is described by interactions between atoms. The MD method consumes much of calculation time if we apply it to larger targets with numerous atoms. To overcome this disadvantage, the acceleration technique of the MD method, RMD method has been presented [Ichishima, 2006]. A renormalization [Rudd, 1998] is a scaling symmetry that actual physical systems have. The RMD method is achieved by the iteration of coarse grainings that preserve the statistical properties of systems between different scales. The coarse graining consists of scaling of momenta, positions, masses and the number of atoms. The RMD method can not only extend the application range of MD, but also provide a new calculating method for partial differential equations (PDEs) without ad-hoc settings of boundary conditions and discontinuous solutions. That is, switching between each phase: solid, liquid and vapor are naturally generated in MD method if the interactions are exact.

On the other hand, macroscopic views are essential in mathematical formulations of PDEs. Although humans recognize a solid object as a subdomain of 3-dimensional space with a boundary, the definition of boundaries for solid objects, i.e., the group of vibrating atoms is not unique. Boundaries are necessary for boundary controls and connecting systems with different scales in the RMD method.

A distributed port-Hamiltonian system [Van der shcaft, 2002] (DPH system) is a framework of boundary controls based on passivity and boundary connections for PDEs [Duindam, 2009]. A DPH system is derived from a Dirac structure [Dorfman, 1993], called a Stokes-Dirac structure [Van der shcaft, 2002]. Dirac structures are generalized symplectic and Poisson structures. Moreover, Stokes-Dirac structures imply boundary integrability in the sense of Stokes theorem. Because of the boundary integrability, the internal energy flow of systems defined on a domain can be transformed into energy flows across the boundary of the domain. In DPH systems, the pair of variables called a boundary port plays the role of boundary input/output variables. We can connect with DPH systems by boundary ports without loss of the consistency with respect to energy. Thus, the DPH system of RMD is used for boundary controls and boundary connections.

This paper is constructed as follows. In Section 2, we

recall RMD methods and extend it to be able to treat higher order potential functions. In Section 3, we first make clear the relationship between continuum mechanics and the DPH system. Then, we introduce the DPH systems of RMD and the boundary power balance of the system. Finally, we will show some numerical examples.

2 Renormalized molecular dynamics method

This section is devoted to explain the fundamentals of the RMD method [Ichishima, 2006].

2.1 MD systems

The Hamiltonian of a monatomic MD is given by

$$H(p,q) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} \sum_{j>i}^{N} \phi(q_{ij}), \tag{1}$$

where $p = (p_1, \cdots, p_N)$, $q = (q_1, \cdots, q_N)$, p_i is the momentum of the i-th particle, q_i is the position of the i-th particle, N is the number of particles, m is a mass, ϕ is a potential function (e.g., see the Lennard-Jones potential for inactive atoms or the Morse potential for metals [Kittel, 2005]), and $q_{ij} = |q_i - q_j|$ is the distance between two particles.

2.2 Statistical equivalence of Hamiltonian systems

Let us consider an MD system governed by a canonical ensemble without quantum effects. In this case, the states of the system can be approximately described by the probability density

$$P = \frac{1}{Z} \exp[-\beta H], \tag{2}$$

$$Z = \frac{1}{N!\, h^{\mu N}} \int_{-\infty}^{\infty} \prod_{i=1}^{N} dp_i\, dq_i \exp[-\beta H], \tag{3}$$

such that $\int_{-\infty}^{\infty} \prod_{i=1}^{N} dp_i\, dq_i\, P(p,q) = 1$, where $\beta = (k_B T)^{-1}$, k_B is the Boltzmann constant, T is the absolute temperature $H(p,q)$ is the (classical) Hamiltonian [Kadanoff, 1999; Huang, 1987], the normalization constant Z is called a partition function, N is the number of particles, μ is the spatial dimension, h is the Planck constant, and the integral is with respect to each p_i and q_i.

The probability density P and the partition function Z yield the statistical properties of the system in thermodynamic equilibrium. Therefore, if the Hamiltonian H is invariant with respect to a certain coarse graining, the systems determined by it are equivalent in the statistical sense under the coarse graining. In the following subsections, we shall describe the way of coarse graining, i.e., transformations of the Hamiltonian.

2.3 Coarse graining of potential energy

Here, we derive the coarse graining of arbitrary higher order potential functions although the original coarse graining is for 3rd order potential functions [Ichishima, 2006]. Removing particle j that lies at the middle point of a line connecting particles i and k can be executed by integrating with respect to the particle j in (3). This reduction can be expressed as scaling transformations of parameters.

Lemma 2.1. *Consider three particles i, j and k lying on a one-dimensional lattice such that the interaction is defined by Hamiltonian (1). Then the following holds:*

$$\int_{-\infty}^{\infty} \exp\left[-\beta\left\{\phi(q_{ij}) + \phi(q_{jk})\right\}\right] dq_j = \Xi_p(u_{ik}) \exp\left[-\beta' \phi\left(\frac{q_{ik}}{2}\right)\right], \tag{4}$$

where $\beta' = 2\beta$ and

$$\Xi_p(u_{ik}) = \sum_{y=1}^{n} \frac{1}{y} \Gamma\left[\frac{1}{2y}\right] (\beta \Psi_{2y})^{-\frac{1}{2y}}, \tag{5}$$

$$\Psi_{2y} = \sum_{s=2y}^{r} (-1)^s 2 \binom{s}{2y} \frac{\phi^{(s)}(a)}{s!} \left(\frac{u_{ik}}{2}\right)^{s-2y} \tag{6}$$

for any integer $r \geq 2$. Here, a is the distance between two lattice points, $u_i = q_i - a_i$ is the displacement from the stable point a_i of particle i, $u_{ij} = u_i - u_j$, Γ is the Gamma function, $\Psi_{2y} > 0$, and integer n is the quotient when r is divided by 2, i.e., $r = 2n$ or $r = 2n+1$.

Proof. Omitted. □

Proposition 2.2. *Let us consider (4). The coefficient $\Xi_p(u_{ik})$ can be considered to be the constant*

$$\Xi_p^0 = \sum_{y=1}^{n} \frac{1}{y} \Gamma\left[\frac{1}{2y}\right] \left(\beta \Psi_{2y}^0\right)^{-\frac{1}{2y}}, \tag{7}$$

$$\Psi_{2y}^0 = 2 \frac{\phi^{(2y)}(a)}{(2y)!}, \tag{8}$$

i.e, $|\Xi_p(u_{ik}) - \Xi_p^0| \ll |\Xi_p^0|$ for all u_{ik} such that $|u_{ik}| \ll a$.

Proof. Omitted. □

Hence, we introduce the following assumption.

Assumption 1. *Systems with N particles are included in a larger uniform system with M particles, where N is even and $M > N$. The coarse graining is applied to the system with M particles.*

From these relations, we can derive the scaling invariance of the potential function.

Theorem 2.3. *Consider N neighboring particles included in a sequence of particles on the one-dimensional lattice. If $|u_{ik}| \ll a$, the following holds:*

$$\int_{-\infty}^{\infty} \prod_{i=1}^{N} dq_i \exp\left[-\beta \sum_{i=1}^{N}\sum_{j>i}^{N} \phi(q_{ij})\right] \propto \int_{-\infty}^{\infty} \prod_{i=1}^{N'} dq_i \exp\left[-\beta' \sum_{i=1}^{N'}\sum_{k>i}^{N'} \phi\left(\frac{q_{ik}}{2}\right)\right], \quad (9)$$

where $N' = 2^{-1}N$ and $\beta' = 2\beta$, and particles $N' + 1, \cdots, N$ have been removed.

Proof. Removing every second particle from the sequence in accordance with *Lemma 2.1* reduces the number of particles by half, so (4) holds for each nearest pair of particles. By *Proposition 2.2*, $\Xi_p(u_{ik})$ in (4) can be considered to be Ξ_p^0 in (8). □

Systems determined by Hamiltonians with the different potential functions in (9) are equivalent in the statistical sense, because the constant coefficients of the probability density (2) are normalized by the partition function (3). This proportional relation can be extended to higher dimensional cases by using the potential moving method [Kadanoff, 1999].

Theorem 2.4 ([Ichishima, 2006]). *A relation corresponding to (9) for the μ-dimensional case is given by $N' = 2^{-\mu}N$ and $\beta' = 2^{\mu}\beta$, where $\mu \geq 1$.*

Remark 2.1. *The condition $\Psi_{2t} > 0$ in Lemma 2.1 is required for the Gauss integral [Gradshteyn and Ryzhik, 2007]. However, we can consider that this condition always holds without loss of generality, because the potential function can be translated by adding constants.*

2.4 Coarse graining of kinetic energy

The coarse graining of kinetic energy is defined by removing a particle and rescaling a momentum of a particle. This reduction can be performed by integrating the relative momentum for a pair of particles.

Lemma 2.5 ([Ichishima, 2006]). *Consider N neighboring particles included in a sequence of particles on the one-dimensional lattice, where the motions of the particles are determined by Hamiltonian (1). Next, we remove every second particle from the set of N particles. Consider three neighboring particles, i, j, and k. We assign $p_k = (p_i + p_j)/2$ to the momentum of particle k after removing particle j. Then the following relation holds:*

$$\int_{-\infty}^{\infty} \prod_{i=1}^{N} dp_i \exp\left[-\beta \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{p_i^2 + p_j^2}{2m}\right] = \Xi_k \int_{-\infty}^{\infty} \prod_{k=1}^{N/2} dp_k \exp\left[-\beta' \sum_{k=1}^{N/2} \frac{p_k^2}{2m}\right], \quad (10)$$

where $\beta' = 2\beta$ and $\Xi_k = (4\pi m/\beta)^{\frac{N}{4}}$.

Theorem 2.6 ([Ichishima, 2006]). *Consider N neighboring particles included in a sequence of particles on a one-dimensional lattice. Then, the following holds:*

$$\int_{-\infty}^{\infty} \prod_{i=1}^{N} dp_i \exp\left(-\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}\right) \propto \int_{-\infty}^{\infty} \prod_{i=1}^{N'} dp_i \exp\left(-\beta' \sum_{i=1}^{N'} \frac{p_i^2}{2m}\right), \quad (11)$$

where $N' = 2^{-1}N$, and $\beta' = 2\beta$.

This transformation is equivalent to the cutting off of high frequency. By repeating the same coarse graining on each spatial axis, the following relation in higher order dimensional space can be derived.

Theorem 2.7 ([Ichishima, 2006]). *A relation corresponding to (11) for the μ-dimensional case is given by $N' = 2^{-\mu}N$ and $\beta' = 2^{\mu}\beta$, where $\mu \geq 1$.*

2.5 Renormalized Hamiltonian systems

We can prove the invariance of the partition function under the above two ways of coarse graining:

$$Z = \frac{1}{N'!\, h^{\mu N'}} \int_{-\infty}^{\infty} \prod_{i=1}^{N'} dp_i\, dq_i \exp\left[-\beta' \sum_{i=1}^{N'} \left\{\frac{p_i^2}{2m} + \sum_{j>i}^{N'} \phi\left(\frac{q_{ij}}{2}\right)\right\}\right], \quad (12)$$

where $N' = 2^{-\mu}N$, $\beta' = 2^{\mu}\beta$, and we have normalized the coefficients Ξ_p^0 and Ξ_k. We can define the following transformation satisfying $dp_i dq_i = dp_i' dq_i'$.

Definition 2.1. *An operator R in a μ-dimensional space is defined as follows:*

$$R\colon (p_i, q_i, m, N) \mapsto (p_j', q_j', m', N') = (2p_j, 2^{-1}q_j, 2^2 m, 2^{-\mu}N), \quad (13)$$

where $\mu \geq 1$, $1 \leq i \leq N$, $1 \leq j \leq N'$, and $i = j$ for $1 \leq j \leq N'$.

In this paper, we assume that the inverse R^{-1} is unique. Finally, the formal system representation is as follows.

Definition 2.2. *A γ-th order renormalized Hamiltonian (RH) system of a monatomic MD determined by (1) in a μ-dimensional space is defined as follows:*

$$\begin{cases} \dfrac{dp'_i}{dt} = -\dfrac{\partial H_\gamma}{\partial q'_i} = -\dfrac{\partial}{\partial q'_i}\displaystyle\sum_{j>i}^{N'} \phi\left(q'_{ij}\right), \\ \dfrac{dq'_i}{dt} = \dfrac{\partial H_\gamma}{\partial p'_i} = \dfrac{p'_i}{m'}, \end{cases} \tag{14}$$

where γ is any integer, and $(p'_i, q'_i, m', N') = (2^\gamma p_i, 2^{-\gamma} q_i, 2^{2\gamma} m, 2^{-\gamma\mu} N)$ for $1 \le i \le N'$ and $H_\gamma(p', q') = H(p, q) \circ R^{-\gamma}(p', q')$ are defined.

3 Boundary power balance of renormalized Hamiltonian systems

RH systems consist of particles; therefore, boundaries of the system cannot be uniquely defined. This section derives the continuum representation RH systems with a unique boundary. The continuum representation is given by the inverse limit of renormalizations in terms of a new scaling, where we assume that a particular coarse-graining rule is given. The boundary is used for defining the boundary power balance of RH systems. The boundary power balance means that the energy variation in an internal system domain is equal to the supplied energy flowing across the boundary of the domain. Hence, the boundary power balance can be applied to boundary energy controls for RH systems.

3.1 Distributed port-Hamiltonian systems

We shall start at the recalling of continuous distributed port-Hamiltonian systems [Van der shcaft, 2002].

Let Z be an n-dimensional smooth manifold with an $(n-1)$-dimensional smooth boundary ∂Z. Let $f^p \in \Omega^p(Z)$, $f^q \in \Omega^q(Z)$, $e^p \in \Omega^{n-p}(Z)$, and $e^q \in \Omega^{n-q}(Z)$, where $\Omega^i(Z)$ is the space of differential i-forms on Z. Then the distributed port-Hamiltonian system is given by

$$\begin{bmatrix} f^p \\ f^q \end{bmatrix} = \begin{bmatrix} 0 & (-1)^r d \\ d & 0 \end{bmatrix} \begin{bmatrix} e^p \\ e^q \end{bmatrix}, \quad \begin{bmatrix} f^b \\ e^b \end{bmatrix} = \begin{bmatrix} e^p|_{\partial Z} \\ (-1)^p e^q|_{\partial Z} \end{bmatrix}, \tag{15}$$

where d is the exterior differential operator, $r = pq+1$, $p + q = n + 1$, and $e^i = \partial\mathcal{H}/\partial\alpha^i$ that means variational derivatives and $f^i = -\partial\alpha^i/\partial t$ are derived from a Hamiltonian density $\mathcal{H}(\alpha^p, \alpha^q) \in \Omega^n(Z)$ for $i \in \{p, q\}$. In (15), f^b and e^b are called boundary port variables, which are a pair of boundary inputs/outputs. Because, f^b and e^b satisfy the following power balance:

$$\int_Z (e^p \wedge f^p + e^q \wedge f^q) + \int_{\partial Z} e^b \wedge f^b = 0 \tag{16}$$

saying that the total energy change of the systems defined within the domain Z with the boundary ∂Z is equal to the energy flowing across the boundary ∂Z.

3.2 Continuum representation of renormalized Hamiltonian systems

Recall the conventional model of continuums derived from ordinary differential equations [Arnold, 1989]. The limit of one-dimensional mass-spring systems can be defined as a continuum; i.e., the transformation of Hamiltonians,

$$\begin{aligned} H_{ms} &= \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N-1} \frac{k}{2}(q_{i+1} - q_i)^2 \\ &\mapsto \mathcal{H}_{ms}\, dx = \left(\frac{1}{2\rho}(\pi^t)^2 + \frac{\kappa}{2}\psi_x^2 \right) dx \end{aligned} \tag{17}$$

is taken to the limits: $a \to 0$, $m \to 0$, $N \to \infty$ and $k \to \infty$ under the constraints: $l = aN$, $\rho = m/a$ and $\kappa = ka$, where we have defined $\psi_t = \partial\psi/\partial t = \lim_{a\to 0} \dot{q}_i$, $\psi_x = \partial\psi/\partial x = \lim_{a\to 0}(q_{i+1} - q_i)/a$ and $\pi^t = \rho\psi_t$, m is the mass, a is the lattice length, l is the length of the system domain $\mathcal{V}$, k is the constant of the spring, $\psi(x, t)$ is the wave function for $x \in \mathcal{V}$, and the Hamiltonian density functional $\mathscr{H}_{ms} = \int_{\mathcal{V}} \mathcal{H}_{ms}\, dx$ is defined by the identification $a = dx$ for an infinitesimal a.

A second-order potential function is used in this interpretation; however, the potential function of RMD is generally of higher order. Furthermore, the lattice length a grows as the number of particles increases. To fill in the differences between the inverse limit of RMD and the conventional continuum limit, we can consider another scaling $\mathcal{S}^\gamma$ of the domain of the RH systems according to the lattice expansion.

Proposition 3.1. *Consider system (14) in a μ-dimensional spatial domain $\mathcal{V}$. Let $\mathcal{S}^\gamma : (q'_i, m') \mapsto (q''_i, m'') = (2^\gamma q'_i, 2^{-\gamma} m')$ for $1 \le i \le N'$ and $H''_{-\infty} = \lim_{\gamma\to-\infty} H_\gamma \circ (\mathcal{S}^\gamma)^{-1}(q''_i, m'')$. We define the (standard) Hamiltonian density and its functional form as follows:*

$$\begin{aligned} H''_{-\infty} &= \mathcal{H}\, dx^{(\mu)} \\ &= \left\{ \frac{1}{2\rho}(\pi^t)^2 + \sum_{s=0}^{r} \Theta_s \left(\psi_x - 1\right)^s \right\} dx^{(\mu)}, \end{aligned} \tag{18}$$

$$\mathscr{H} = \int_{\mathcal{V}''} \mathcal{H}\, dx^{(\mu)}, \tag{19}$$

where t is the time coordinate, $x = (x^1, \cdots, x^\mu)$ is the set of spatial coordinates,

$$\pi^t = \lim_{\gamma\to-\infty} \rho\, \dot{q}_i, \quad \psi_{x^l} = \lim_{\gamma\to-\infty} \frac{\tau_l q_{ij}}{2^\gamma a}, \tag{20}$$

$$\Theta_s = \lim_{\gamma\to-\infty} \left[\frac{\phi_\gamma^{(s)}(2^\gamma a)}{s!} (2^\gamma a)^{s-\mu} \right], \tag{21}$$

$\rho = 2^{\gamma} m/(2^{\gamma}a)^{\mu}$, $\tau_l q_{ij}$ is the variable in the direction of axis X_l in hypercubic coordinates, ψ_{x^l} is the partial derivative of ψ with respect to x^l, $\psi_x = (\psi_{x^1}, \cdots, \psi_{x^\mu})$, $\mathcal{V}''$ is the system domain $\mathcal{V}$ scaled by $\mathcal{S}^{\gamma}$, and $dx^{(\mu)} = (2^{\gamma}a)^{\mu}$ is defined for an infinitesimal $2^{\gamma}a$ when $\gamma \to -\infty$.

Proof. The size of the domain re-scaled by $\mathcal{S}^{\gamma}$ is invariant with respect to R^{γ}, because $2^{\gamma}q' = 2^{\gamma}2^{-\gamma}q = q$. The potential function $\phi(q_{ij}) = \sum_{s=0}^{r}(\phi^{(s)}(a)/s!)(q_{ij}-a)^s$ for neighboring particles i and j is scaled by $\mathcal{S}^{\gamma}$ as follows:

$$\phi_{\gamma}(2^{\gamma}q'_{ij}) = \sum_{s=0}^{r} \frac{\phi_{\gamma}^{(s)}(2^{\gamma}a)}{s!} (2^{\gamma}a)^s \left(\frac{2^{\gamma}q'_{ij}}{2^{\gamma}a} - 1\right)^s, \tag{22}$$

$$\lim_{\gamma \to -\infty} \phi_{\gamma}(2^{\gamma}q'_{ij}) = \sum_{s=0}^{r} \Theta_s \left(\psi_x - 1\right)^s \, dx^{(\mu)}, \tag{23}$$

where $q'_{ij} = 2^{-\gamma}q_{ij}$ and the stable point of ϕ_{γ} is $2^{\gamma}a$; i.e., ϕ_{γ} is a horizontally scaled function of ϕ, and the kinetic energy function is scaled as follows: $p_i''^2/(2m'') = (2^{-\gamma}m'2^{\gamma}q'_i)/\{2(2^{-\gamma}m')\} = p_i'^2/\{2(2^{-\gamma}m')\} = (\pi^t)^2(2^{\gamma}a)^{\mu}/(2\rho)$, where $m' = 2^{2\gamma}m$ and $\rho = 2^{-\gamma}m'/(2^{\gamma}a)^{\mu}$. By substituting (21) into these functions, we get (19). □

3.3 Boundary power balance of renormalized Hamiltonian systems

From the scaled Hamiltonian (19), we obtain the following standard representation for boundary energy controls.

Proposition 3.2. *Let $\mathcal{V}''$ be a μ-dimensional connected compact submanifold of $\mathbb{R}^{\mu}$ with a boundary $\partial\mathcal{V}''$. Consider the Hamiltonian density functional in (19). Then, the following distributed port-Hamiltonian system [Van der shcaft, 2002] can be derived from (19):*

$$\begin{bmatrix} f_p \\ f_q \end{bmatrix} = \begin{bmatrix} 0 & d \\ (-1)^{\xi} d & 0 \end{bmatrix} \begin{bmatrix} e_p \\ e_q \end{bmatrix}, \quad \begin{bmatrix} f_b \\ e_b \end{bmatrix} = \begin{bmatrix} e_p|_{\partial\mathcal{V}''} \\ -e_q|_{\partial\mathcal{V}''} \end{bmatrix}, \tag{24}$$

where $\xi = \mu + 1$,

$$\begin{cases} f_p = -\dfrac{\partial}{\partial t}\pi^t = -\dfrac{\partial}{\partial t}(\rho\psi_t)\, dx^{(\mu)}, \\ f_q = (-1)^{\xi}\dfrac{\partial}{\partial t}\dfrac{\partial \mathcal{H}}{\partial \pi^x} = (-1)^{\xi}\dfrac{\partial}{\partial t}\psi_x \, dx^{(1)}, \\ e_p = \dfrac{\partial \mathcal{H}}{\partial \pi^t} = \psi_t, \\ e_q = \pi^x = -\displaystyle\sum_{s=1}^{r} s\Theta_s \left(\psi_x - 1\right)^{s-1} dx^{(\mu-1)}, \end{cases} \tag{25}$$

t is the time coordinate, $x = (x^1, \cdots, x^{\mu})$ is the set of spatial coordinates, r is a positive integer, $dx^{(k)}$ is a differential k-form defined on $\mathbb{R}^{\mu}$, and $\mathcal{H}(\psi, \pi^i) = \pi^i\psi_i - \mathcal{L}(\psi, \psi_i)$ and $\pi^i = \partial\mathcal{L}(\psi, \psi_i)/\partial\psi_i$ for $i \in \{t, x\}$ are defined. The system (24) with variables (25) satisfies the following boundary power balance:

$$\int_{\mathcal{V}''} (e_p \wedge f_p + e_q \wedge f_q) + \int_{\partial\mathcal{V}''} e_b \wedge f_b = 0, \tag{26}$$

which means the energy variation in the internal domain $\mathcal{V}''$ is equal to the energy flowing across the boundary $\partial\mathcal{V}''$.

Proof. The proof is by direct calculation. First, (24) is the formal form of distributed port-Hamiltonian systems [Van der shcaft, 2002] in the case of $p = \mu$ and $q = 1$. In the first equation of (24), the first row $f_p = de_q$ is equivalent to the Euler-Lagrange equation,

$$\left\{ \frac{\partial}{\partial t}(\rho\psi_t) - \sum_{i=1}^{\mu} \frac{\partial}{\partial x^i} \left(\sum_{s=1}^{r} s\Theta_s \left(\psi_x - 1\right)^{s-1} \right) \right\} dx^{(\mu)} = 0, \tag{27}$$

which is the dual expression of the scaled Hamiltonian system $v_{-\infty} = \mathcal{F}_{-\infty} d(H''_{-\infty})$, and the second row is the identity, where the second term of (27) is equal to de_q,

$$\sum_{i=1}^{\mu} \frac{\partial}{\partial x^i} \left(\sum_{s=1}^{r} s\Theta_s \left(\psi_x - 1\right)^{s-1} \right) dx^{(\mu)} = d\left(\sum_{s=1}^{r} s\Theta_s \left(\psi_x - 1\right)^{s-1} dx^{(\mu-1)} \right), \tag{28}$$

which comes from integration by parts in the variational calculus of $\mathcal{L}(\psi, \psi_i)$. Equation (26) was proven by means of Stokes theorem in [Van der shcaft, 2002]. Here, we check the relation between (26) and the Hamiltonian density in (19). Indeed, the energy variation of (24) can be derived from

$$\begin{aligned} & e_p \wedge (-f_p) + e_q \wedge (-f_q) \\ &= \frac{\partial}{\partial t}\pi^t \frac{\partial \mathcal{H}}{\partial \pi^t} dx^{(\mu)} - \pi^x \frac{\partial}{\partial t}\frac{\partial \mathcal{H}}{\partial \pi^x} dx^{(1)} \wedge dx^{(\mu-1)} \\ &= \boldsymbol{i}_{\mathcal{X}} d\mathcal{H}\, dx^{(\mu)}, \end{aligned} \tag{29}$$

where $i \in \{t, x\}$, $\boldsymbol{i}_{\mathcal{X}}$ is the interior product with respect to the vector field $\mathcal{X} = (\partial\pi^i/\partial t)(\partial/\partial\pi^i) + (\partial\psi/\partial t)(\partial/\partial\psi)$, $d\mathcal{H} = (\partial\mathcal{H}/\partial\pi^i)d\pi^i + (\partial\mathcal{H}/\partial\psi)d\psi$, $\partial/\partial t\left(\pi^i\psi_i\right) = 0$, and $\partial\mathcal{H}(\psi, \pi^i)/\partial\pi^i = \psi_i$. Hence, the energy variation is the time derivative of an energy function. □

The variables e_q and e_p in (25) have the dimensions of force and velocity. The product $e_q \cdot e_p$ is power. The variables e_q and e_p for the particles $i, j \in \partial V_{\gamma}$ are used as the input and output called *boundary ports* for the

passivity-based boundary controls. Typical passivity-based boundary controls are shaping Hamiltonians and damping assignments [Van der Schaft, 2000; Duindam, 2009]. The former means connecting controllers to change Hamiltonians by means of boundary ports. The latter means stabilizing the system to the global minimum of the shaped Hamiltonian by assigning velocity feedbacks to the ports. These methods make systems robust against disturbances.

4 Numerical calculations

4.1 Computing environment

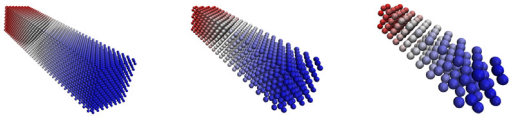
We carried out RMD methods by using the host computer (Dual Xeon X5492 3.4GHz) with the acceleration board MDGRAPE-3 (MD3-PCIX) [MDGRAPE-3, RIKEN] (Fig.1) with MDGRAPE-3 chip developed by Hitachi Device Development Center (Fig.2).

Fig. 1. MDGRAPE-3 (MD3-PCIX)

Fig. 2. MDGRAPE-3 chip

4.2 Numerical experiment of bending of Aluminum bar with RMD methods

We used the Aluminum bar with 9.44×10^{21} atoms in $33.5 \times 6.35 \times 6.35$ [mm^3], where the crystal is face-centered cubic. After 21, 22 and 23 renormalizations, the numbers of atoms become 10240, 1280 and 160, respectively (see Fig.3 visualized by VMD [VMD, Univ. of Illinois]).



10240 atoms 1280 atoms 160 atoms

Fig. 3. Renormalized aluminum bars

The performed times per the calculation time 5.0×10^{-5} [sec] are 12.3, 8 and 5 [sec] for the cases of 21, 22 and 23 renormalizations, respectively. We considered the Timoshenko beam model, where the Young's modulus is 7.03×10^{10} [Pa], the shear modulus is 2.61×10^{10} [Pa], and the section of area is square.

Fig.4 shows the comparisons with the theoretical solution of the Timoshenko beam model. In Fig.4, the horizontal axis means the longitudinal coordinate, the vertical axis means the lateral coordinate, the solid line means the strain of the beam, and round points, square points and diamond points correspond to the cases of 21, 22 and 23 renormalizations, respectively. We can see that the approximate strains are reproduced by the RMD method except the case of 160 atoms.

In Fig.5, the horizontal axis means the time evolution, the vertical axis means the amplitude of vibrations, we see that the eigenfrequency of Timoshenko beam model is 2.9×10^4 [rad/s], and that of the case of 10240 atoms is 2.61×10^4 [rad/s]. However, the results of 160 atoms are beyond the limits of measurements, because the crystal structure was broken up by large dynamical motions. As the number of atoms decreases, the eigenfrequency becomes lower than the theoretical value, because higher frequency modes might be eliminated by the renormalization.

Fig.6 shows the time response of the strain of the controlled beams in the case of 10240 atoms. We applied a boundary energy control, i.e., assigning dampings to the boundary ports distributed on an area at the both sides of beam. We can see that the beam is stabilized.

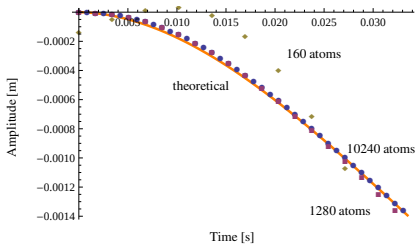


Fig. 4. Time response of strains with loads

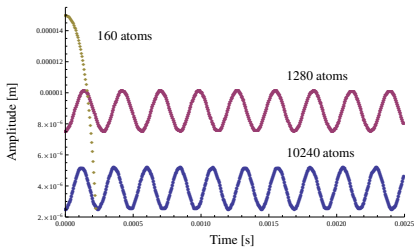


Fig. 5. Time response of free vibrations

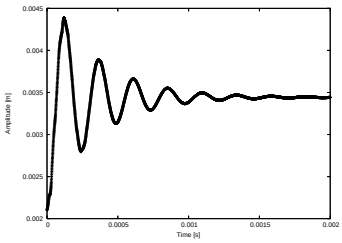


Fig. 6. Time response of strain with control

5 Conclusion

This paper derived the distributed port-Hamiltonian (DPH) systems of renormalized molecular dynamics (RMD) that is expected as a unified framework of boundary controls and numerical calculus. The DPH system of RMD is scale-free, i.e., we can apply this representation not only to microscopic targets like polymers, but also macroscopic targets like mechanical systems. First, we introduced renormalized Hamiltonian systems. Next, we derived the continuum representation of renormalized Hamiltonian systems from the inverse limit of coarse graining. As a result, we derived a standard boundary control representation of renormalized Hamiltonian systems from DPH systems. Finally, we will show some numerical examples.

We can connect DPH systems by means of boundary ports on their common boundaries. Conversely, we divide a DPH system into uniform subsystems by creating boundaries and boundary ports of each subsystem. Thus, DPH systems provide us the freedom of meshing of continuum mechanics. The structure of the connection can be described by bond graph theory [Karnopp, 2006]. We are interested in the developments of the DPH systems in terms of such a freedom of meshing and parallel computations as more useful numerical tools.

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