ACCURATE BOUNDARY CONDITIONS FOR ONE-DIMENSIONAL ATOMIC CHAINS

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Summary In this paper, we design a class of accurate boundary conditions for one-dimensional atomic chain, based on matching the kernel functions. Taking the form of a linear constraint among the displacements and relations near the boundary, the proposed conditions are local in space and time. Consequently, we completely resolve the heavy computing loads while retaining the same accuracy as the time history kernel treatment, and avoid long time reflection due to the time cut-off.

INTRODUCTION

We consider an infinite one-dimensional harmonic lattice. When a finite segment is computed numerically, artificial boundary conditions are needed at the numerical boundary atom. The fundamental issue in designing such a boundary condition is the reconstruction of the evolution for the boundary atom from information of the interior atoms.

ARITIFIAL BOUNDARY CONDITION FOR ONE-DIMENSIONAL ATOMIC CHAIN

Kernel Function for One-Dimensional Atomic Chain

If there is a single source at an interior atom, e.g., $u_0(t) = f(t)$ whereas all other atoms are at equilibrium initially, then it is known that

$$u_n(t) = g_n(t) * f(t), \text{ for } n \geq 1,$$

with the kernel function $g_n(t) = \dfrac{2nJ_{2n}(2t)}{t}$. Here $J_n(t)$ is the first kind of Bessel function.

The time history kernel method then follows with $u_N(t) = g_1(t) * u_{N-1}(t)$. That is, one may reconstruct the displacement at the boundary atom $u_N(t)$ from the time history of $u_{N-1}(t)$. Being an exact boundary condition for semi-infinite segment simulations, the heavy computing load in the time convolution and non-locality restrict the reflection suppression of this treatment, particularly for nonlinear problems and in multiple dimensions. Hence we seek for local and accurate boundary conditions from another perspective.

Matching Coefficients and Constricting Artificial Boundary Condition

From lengthy manipulations, we discover the following properties of the Bessel functions.
For fixed p, large N and $N - p \leq k \leq N - 1$, we have

$$J_k(t) \approx \begin{cases} F_{1,\,k}(t^2 - k^2), & t \in [0, N - AN^{\frac{1}{3}}] \\ F_{2,\,k}(t^2 - k^2), & t \in [N - AN^{\frac{1}{3}}, \dfrac{3}{2}N] \\ F_{3,\,k}(t^2 - k^2), & t \in [\dfrac{3}{2}N, \infty) \end{cases} \tag{1}$$

where $F_1(x)$, $F_2(x)$, $F_3(x)$ are all power series or oscillating asymptotic series with respect to x.
We make an approximation

$$g_N(t) \approx \sum_{k=1}^{p} a_k g_{N-k}(t) + \sum_{k=1}^{p} b_k \dot{g}_{N-k}(t). \tag{2}$$

Expanding $F_{1,k}(t^2 - k^2)$, $F_{2,k}(t^2 - k^2)$, $F_{3,k}(t^2 - k^2)$ in terms of $t^2 - N^2$, and equating the coefficients of both sides of (2), we calculate the coefficients a_k and b_k. This leads to an accurate boundary condition as follows.

$$u_N = \sum_{k=1}^{p} a_k u_{N-k} + \sum_{k=1}^{p} b_k \dot{u}_{N-k}\ . \tag{3}$$

It is local in both space and time. The accuracy relies on the quality of the approximation (2).

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NUMERICAL RESULTS

We demonstrate that the approximation may be worked out with high accuracy by an example. Take $N = 75$, and $p = 12$. By suitably taking the coefficients, the optimal matching is depicted in Figure 1. Comparing the solid line for $g_N(t)$ and circles for $\sum_{k=1}^{p} a_k g_{N-k}(t) + \sum_{k=1}^{p} b_k \dot{g}_{N-k}(t)$, we observe an excellent coincidence.

Furthermore, using the accurate boundary condition for the atomic simulation of a harmonic chain, the reflection is better suppressed than existing methods, such as the matching boundary condition and the time history kernel method [1,2]. We notice that the computational cost is comparable to the matching boundary condition, which is much less than the time history kernel method.

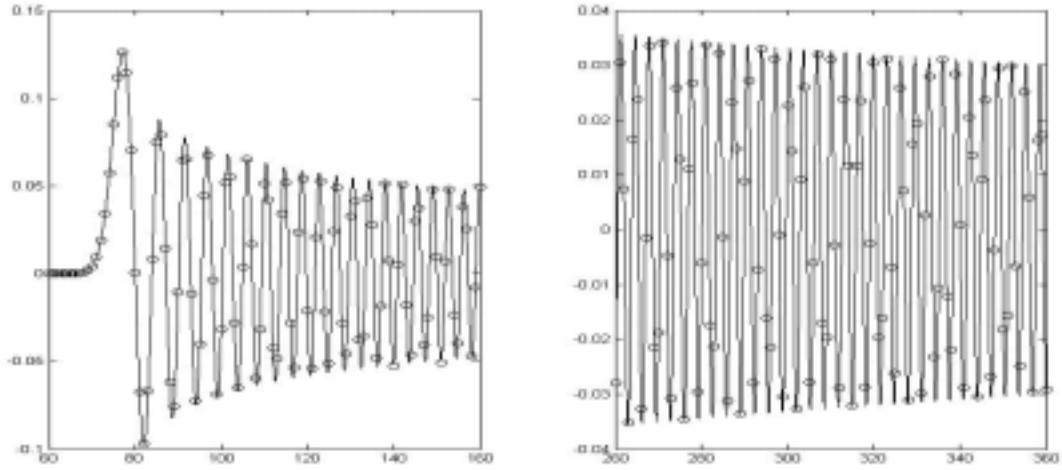

Figure 1. Matching of the kernel functions.

CONCLUSIONS

In this paper we propose an accurate artificial boundary condition for one-dimensional chain, based on matching the kernel functions. While retaining the high accuracy of the time history kernel method, the proposed condition is local in space and time, hence more effective and applicable to nonlinear chains and multi-scale simulations with high accuracy.

References

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[2] Wang X, Tang S: Matching boundary conditions for diatomic chains. Computational Mechanics, 46: 813—826 2010.