MESH PARTITIONING FOR HPX PARALLEL COMPUTING FOR NONLOCAL COMPUTATIONAL MODELS

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In this document, we consider a general class of nonlocal computational model seen in various fields, such as Peridynamics [21, 4, 14, 1, 12, 8, 19, 16, 17], discrete element method [6, 7, 13, 20, 9], Peridynamics plus discrete element method for granular media [26, 3], nonlocal cell-cell adhesion in computational biology [2, 11, 22], nonlocal heat equation [5, 10]. References above are only minuscule fraction of what is available. The application of nonlocal modeling method for understanding of complex spatially multiscale phenomenon is seen in various new fields such as fluid mechanics, particulate media, directed self-assembly of Block-Copolymers, tumor modeling, etc. What is more interesting and also convenient is that underlying algorithm which is used to numerically solve these nonlocal models is more or less same and therefore the efficient computational method available for one type of nonlocal model can be easily applied to the nonlocal model in other fields.

It is our understanding that efficient computational method to solve the nonlocal model is very important. It is widely known that the nonlocal models are much more computationally demanding compared to their counterpart, namely local models (such as heat equation, wave equation, etc). This is because the length of interaction in nonlocal model is typically 3 to 10 times larger than the size of discretization and therefore, the usual local assembly of matrix and vector considered in solution of pdes (partial differential equation) is not feasible. The efficient parallel implementation because of long-range interaction is difficult due to dependence over much larger length scale.

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In this document we present this problem using simple example of nonlocal diffusion equation, see [5] and references therein for more information. Our main goal is to highlight key difficulties in designing massively parallel scheme for nonlocal models while keeping the model related complexity to minimum. For this purpose nonlocal heat equation is suitable. Further, to fix the ideas we only consider two dimensional setting.

In this work we use parallel API called HPX. HPX is an open source asynchronous many task run time system that focuses on high performance computing [15, 23, 18]. HPX provides wait-free asynchronous execution and futurization for synchronization. It also features parallel execution policies utilizing a task scheduler, which enables a fine-grained load balancing parallelization and synchronization due to work stealing. HPX is in strict adherence to the C++ 11 [24] and C++ 17 standard definitions [25].

1. Nonlocal diffusion equation

In this section we give brief overview of nonlocal diffusion equation for temperature field u over an square domain $D = [0,1]^2$ subjected to zero temperature condition on its boundary and subjected to given heat source distribution within the domain. It is a first order transient equation in time. For simplification, we only consider explicit time integration scheme, namely forward Euler scheme. For spatial discretization, we consider uniform mesh over domain D and consider finite difference approximation (also commonly referred to as particle discretization). The resulting final equations are very simple and serial implementation requires only few lines of code, see 1. With HPX, thread-level parallel implementation and shared-memory parallel implementation is almost as simple as serial implementation, see 2.

Our goal is to fully parallelize the solver, i.e. starting from mesh partition to computation of fields at mesh nodes. We proceed step wise starting from serial implementation, to shared-memory parallel implementation, and to fully parallel implementation and discuss the challenges going from one step to next.

Let material domain is $D = [0,1]^2$ and time domain $I = [0,T]$. We fix size of horizon (length over one point interacts with another, also called nonlocal length scale) $\epsilon > 0$. Let $D_c = (-\epsilon, 1+\epsilon)^2 - D$ be the nonlocal boundary of thickness ϵ surrounding D. See Figure 1. We define $H_r(x)$ as two-dimensional open ball of radius r centered at $x \in \mathbf{R}^2$.

Let $u : I \times D \cup D_c \to \mathbf{R}$ is a temperature field. Let $J : \mathbf{R} \to \mathbf{R}$ be positive function such that $0 \leq J(r) \leq M$

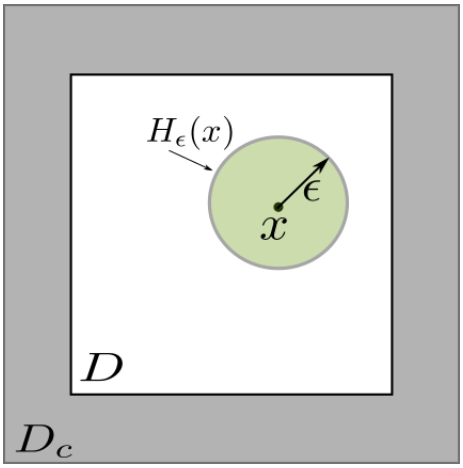

FIGURE 1. Material domain D and nonlocal boundary D_c. Figure shows typical material point $x \in D$ and ball $H_\epsilon(x)$.

for $r \in [0,1]$ and $J(r) = 0$ for $r \notin [0,1]$. We refer to J as influence function.

$u(t,x)$ satisfies following nonlocal diffusion equation, $\forall x \in D$ and $\forall t \in I$,

$$\partial_t u(t,x) = b(t,x) + c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})(u(t,y)-u(t,x))dy, \tag{1.1}$$

where $b(t,x)$ is the external source at time t and at point x (this is a known function of space and time). Initial condition is given by

$$u(0,x) = u_0(x) \qquad \forall x \in D \tag{1.2}$$

and boundary condition is given by

$$u(t,x) = 0 \qquad \forall x \in D_c \text{ and } \forall t \in I. \tag{1.3}$$

Constant c is chosen such that in the limit $\epsilon \to 0$ the nonlocal operator in right-hand side of Equation 1.1. goes to $k\nabla \cdot \nabla u$. Local diffusion equation is given by

$$\partial_t u(t,x) = k\nabla \cdot \nabla u(t,x), \tag{1.4}$$

where k is the diffusivity constant. Boundary condition is $u = 0$ on ∂D (consistent with boundary condition in Equation 1.3 and initial condition is $u(0,x) = u_0(x)$. Constant c is taken as

$$c := \begin{cases} \frac{k}{\epsilon^3 M_2}, & \text{when dimension } d = 1 \\ \frac{2k}{\pi\epsilon^4 M_3}, & \text{when dimension } d = 2, \end{cases} \tag{1.5}$$

where

$$M_i = \int_0^1 J(r) r^i dr. \tag{1.6}$$

For standard influence functions, M_i can be computed easily. For example, when $J = 1$, $M_i = 1/(i+1)$, when $J = 1 - r$, $M_2 = 1/12, M_3 = 1/20$, etc.

With choice of constant c in Equation 1.5, it can be shown formally (see Appendix B) that

$$c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})(u(t,y)-u(t,x))dy \to k\nabla \cdot \nabla u(t,x). \tag{1.7}$$

Algorithm 1 Serial implementation

```
% Create neighbor list
for each integer i ∈ K do
    if |x_i − x_j| ≤ ε then
        Add j to neighborList[i]
    end if
end for

% U is the vector of temperatures of
% all mesh nodes.

% integrate in time
for each integer 0 ≤ k ≤ T/Δt do
    % time step k
    for each integer i ∈ K do
        % Loop over neighbors of i
        val_i = 0
        for each integer j ∈ neighborList[i] do
            val_i = val_i+
                cJ(|x_j − x_i|/ε)(U[j] − U[i])V_j
        end for
        % get external source
        b_i = b(t^k, x_i)
        % Update temperature
        U[i] = U[i] + Δt × val_i + Δt × b_i
    end for
    % Output temperature at time t^k = kΔt
    Output(U)
end for
```

2. Finite difference approximation

Consider uniform mesh $D_h = (D \cup D_c) \cap (h\mathbf{Z})^2$ of mesh size $h > 0$, see Figure 2. $\mathbf{Z}$ is the set of positive and negative integers. Let Δt is size of time step and $[0,T] \cap (\Delta t\mathbf{Z})$ be the discretization of time domain. We assume $\epsilon = mh$ where $m \geq 1$ is some integer.

We consider index set $K \subset \mathbf{Z}^2$ such that for $i \in K$, $x_i = hi \in D$. Similarly, consider index set $K_c \subset \mathbf{Z}^2$ such that for $i \in K_c$, $x_i = hi \in D_c$.

Let $\hat{u}_i^k$ be the solution of forward Euler discretization in time. It satisfies,$\forall 1 \leq k \leq T/\Delta t, \forall i \in K$,

$$\frac{\hat{u}_i^{k+1} - \hat{u}_i^k}{\Delta t} = b(t^k, x_i) + c\sum_{\substack{j \in K \cup K_c, \\ |x_j - x_i| \leq \epsilon}} J(|x_j - x_i|/\epsilon)(\hat{u}_j^k - \hat{u}_i^k)V_j \tag{2.1}$$

and

$$\hat{u}_i^k = 0 \qquad \forall 0 \le k \le T/\Delta t, \forall i \in K_c. \tag{2.2}$$

At $k = 0$, we have $\hat{u}_i^0 = u_0(x_i)$ for all $i \in K$. V_j is the volume occupied by node j and in our case we have $V_j = h^2$.

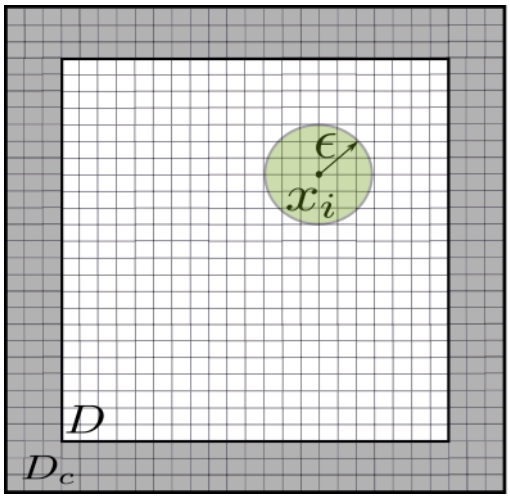

FIGURE 2. Uniform mesh of size h. Shaded area corresponds to nonlocal boundary D_c. We specify zero temperature on all the mesh nodes in the shaded area. For mesh node x_i in D, we consider interaction of x_i with all the mesh nodes inside the green shaded ball.

2.1. **Serial and semi-parallel implementation of forward euler scheme.** Algorithm for serial implementation is given in Algorithm 1. For parallel implementation, we will use parallel for loop (HPX utility). See Algorithm 2. In Algorithm 2, we observe that temperature data of all mesh nodes is stored in single data variable, "U", and similarly, neighbor list of all the mesh nodes are stored in single data variable, "neighborList". We refer to this as semi-parallel as we have only parallelized for-loop and not the data. In fully parallel implementation, data will also be divided in number of computational nodes and each computational node will own data corresponding to it. This requires mesh partition. We discuss this in next section.

3. Parallelization and mesh partition

Given N number of computational nodes, mesh will be partitioned in N parts such that each computational node will store the information corresponding to the mesh partition it owns. For example, consider 4 computers connected by network. We would like to run the problem on all 4 computers in parallel. We will partition the mesh in four parts, see Figure 3.

In Figure 3, the mesh is colored to show the partition. Consider part of mesh colored as green. Let us suppose

Algorithm 2 Semi-parallel implementation

```
% Create neighbor list using
% hpx parallel for loop
hpx::parallel::for_loop each integer i ∈ K do
  if |x_i − x_j| ≤ ε then
    Add j to neighborList[i]
  end if
end parallel for

% is the vector of temperatures of
% all mesh nodes.

% integrate in time
for each integer 1 ≤ k ≤ T/Δt do
  % time step k
  % process mesh nodes in parallel
  hpx::parallel::for_loop each integer i ∈ K
    % Loop over neighbors of i
    val_i = 0
    for each integer j ∈ neighborList[i] do
      val_i = val_i+
        +cJ(|x_j − x_i|/ε)(U[j] − U[i])V_j
    end for
    % get external source
    b_i = b(t^k, x_i)
    % Update temperature
    U[i] = U[i] + Δt × val_i + Δt × b_i
  end parallel for
  % Output temperature at time t^k = kΔt
  Output(U)
end for
```

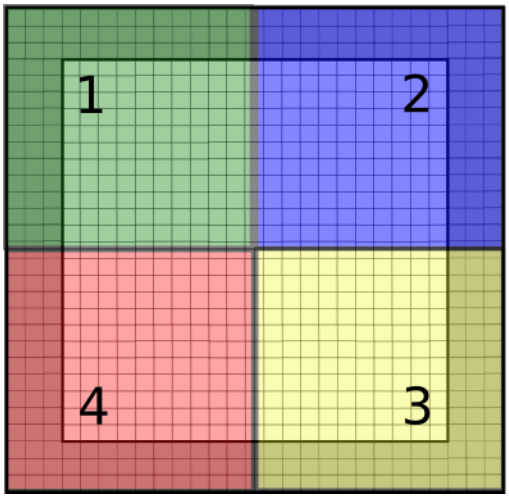

FIGURE 3. Typical mesh partition. Mesh nodes under each color are owned by the respective computer.

the id of computer who owns the green, blue, yellow, and red are 1, 2, 3, and 4 respectively. We now focus on one computational node, say green, and present two possible situations.

Case 1: Consider mesh node x_i which belongs to computer 1's partition. Let us suppose that x_i is within the dashed line, see Figure 4. For such x_i, all mesh nodes $x_j \in H_\epsilon(x_i)$ will be within the green partition. Since computer 1 owns the mesh data of green partition, calculation of right hand side of Equation 2.1, i.e. $cJ(|x_j - x_i|/\epsilon)(\hat{u}_j^k - \hat{u}_i^k)V_j$, can be carried out without needing to interact with other computers.

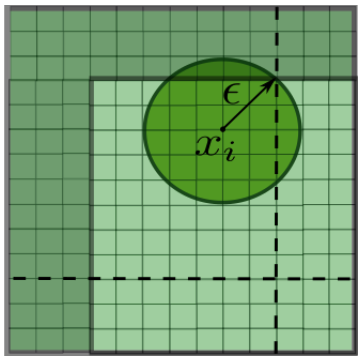

FIGURE 4. Mesh nodes of green partition which are within dashed line do not interact with partition owned by other computers.

Case 2: Now consider another mesh node x_i in green partition. This mesh node is close to the boundary of green partition, and we see that there are mesh nodes x_j which are in ball $H_\epsilon(x_i)$, but which are not part of green partition. For example, we consider $x_j \in H_\epsilon(x_i)$ in Figure 5. Mesh node x_j is in Blue partition. Blue partition is owned by computer 2. Therefore, to compute the right hand side term in Equation 2.1, computer 1 has to request the information associated to mesh node x_j from computer 2. We see that for all the mesh nodes in Green partition which are outside dash line, computer 1 will have to communicate with other computers for the information.

3.1. **Algorithm for fully parallel code.** Consider Algorithm 3 which outlines the steps needed to run the problem in fully parallel framework. Following are the list of steps which will require effort in implementing Algorithm 3.

1. Partitioning of mesh: Libraries are available which can partition the mesh into given number of computational nodes.

2. List of interacting mesh nodes owned by other computational node: If global mesh data is available to each computational node then we can create a list of interacting neighboring mesh nodes which are owned by other computational node. This list will have global id, which is unique, of mesh nodes.

3. Sharing of information: For given computational node, we need to implement the method which shares information to other computational node and which receives the information from other computational node.

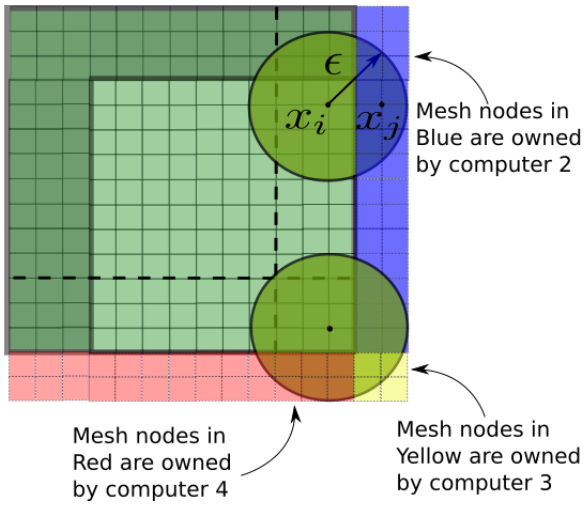

FIGURE 5. In first example, mesh node x_i of Green partition interacts with few mesh nodes of Blue partition owned by computer 2. In second example, we see that x_i of Green mesh interacts with mesh nodes owned by computer 2, 3, and 4.

For this we need a list of information to be shared and communication method available in HPX framework.

Algorithm 3 Fully parallel implementation

```
% mesh_file is the file containing mesh data
% N is the number of computational nodes

% get the id of this computational node
my_id = get_id()

% read mesh data and create mesh partition
myMeshNodes = create_mesh_partition(mesh_file)

% create neighbor list.
neighborList = create_neighbor_list(mesh_file)

% next task is to create a list of mesh
% nodes, associated to other computational
% nodes, which interact with mesh nodes
% owned by this computational node
for each integer 0 ≤ i ≤ N do
  if i == my_id then
    % skip this i
  else
    % create a list of interacting nodes
    % owned by comp. node i
    neighborsOutside[i]
      = create_list_interacting_nodes(my_id, i)
  end if
end for

% U is the vector of temperatures of
% mesh nodes owned by this comp. node

% integrate in time
for each integer 0 ≤ k ≤ T/Δt do
  % time step k

  % get data from other computer
  % before integrating in time
  for each integer 0 ≤ i ≤ N do
    if i == my_id then
      % skip this i
    else
      % request data from comp. node i
      getData[i] = request_data(my_id, i)

      % share data to comp. node i
      % as comp. node i may also have
      % mesh nodes which have neighbors
      % in this comp. node
      share_data(my_id, i)
    end if
  end for

  % we now have all the relevant data so
  % we can solve for temperature
  % at next time step
  hpx::parallel::for_loop i ∈ myMeshNodes do
    % Loop over neighbors of i
    val_i = 0
    for each integer j ∈ neighborList[i] do
      % check if j is in myMeshNode
      if j ∈ myMeshNode then
        % this mesh node is within dashed line

        % compute contribution
        val_i = val_i
          +cJ(|x_j − x_i|/ϵ)
          (U[j] − U[i])V_j
      else
        % this mesh node is outside dashed line
        % search and find which comp. node
        % owns mesh node j
        get_comp_id =
          search_for_mesh_node(my_id, j)

        % Look for j in getData[get_comp_id]
        % and get the temperature of mesh node j
        t_j = find_in(j, getData[get_comp_id])

        % compute contribution
        val_i = val_i
          +cJ(|x_j − x_i|/ϵ)
          (t_j − U[i])V_j
      end if
    end for
    % get external source
    b_i = b(t^k, x_i)
    % Update temperature
    U[i] = U[i] + Δt × val_i + Δt × b_i
  end parallel for
  % Output temperature at time t^k = kΔt
  Output(U)
end for
```

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A. Constructing exact solution

The idea is to use source term b to construct the analytical solution. This is shown next.

A.1. One dimension.

Let

$$w(t,x) = \cos(2\pi t)\sin(2\pi x)$$

when $x \in [0,1]$ and $w(t,x) = 0$ when $x \notin [0,1]$. We want solution of Equation 1.1 u to be equal to w, i.e., $u = w$. To achieve this we substitute

$$b(t,x) = \partial_t w(t,x) - c\int_{H_\epsilon(x)} J(|y-x|/\epsilon)(w(t,y)-w(t,x))dy \tag{A.1}$$

in Equation 1.1 and prescribe $u(0,x) = w(0,x) = \sin(2\pi x)$ as initial condition on u and $u(t,x) = 0$ on $x \in D_c$ as boundary condition. Note that

$$\partial_t w(t,x) = -2\pi\sin(2\pi t)\sin(2\pi x)$$

when $x \in [0,1]$ and $\partial_t w(t,x) = 0$ when $x \notin [0,1]$.

A.2. Two dimension.

Let

$$w(t,x) = \cos(2\pi t)\sin(2\pi x_1)\sin(2\pi x_2)$$

when $x \in [0,1]^2$ and $w(t,x) = 0$ when $x \notin [0,1]^2$. We substitute

$$b(t,x) = \partial_t w(t,x) - c\int_{H_\epsilon(x)} J(|y-x|/\epsilon)(w(t,y)-w(t,x))dy \tag{A.2}$$

in Equation 1.1 and prescribe

$$u(0,x) = w(0,x) = \sin(2\pi x_1)\sin(2\pi x_2)$$

as initial condition on u and $u(t,x) = 0$ on $x \in D_c$ as boundary condition.

To obtain numerical solution $\hat{u}_i^k$ following discretization Equation 2.1, we essentially have to compute source b at time $t = t^k = k\Delta t$ and point $x = x_i = ih$ using the formula Equation A.1 (in 1-d simulation) and Equation A.2 (in 2-d simulation).

A.3. Numerical discretization error.

Suppose $\bar{u}(t,x)$ is the exact solution and $\hat{u}_i^k$ for $0 \le k \le T/\Delta t$ and $i \in K$ is the numerical solution. The total error at time t^k is taken as

$$e^k := h^d \sum_{i\in K} |\bar{u}(t^k,x_i) - \hat{u}_i^k|^2, \tag{A.3}$$

where $d = 1, 2$ is the dimension. Total error can be defined as $e := \sum_{0\le k\le T/\Delta t} e^k$.

B. Limit of nonlocal operator to local operator in diffusion equation

We show through formal calculation that

$$c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})(u(y)-u(x))dy \to k\nabla\cdot\nabla u(x).$$

Let

$$\mathcal{L}(u)(x) = c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})(u(y)-u(x))dy, \tag{B.1}$$

where

$$c := \begin{cases} \frac{k}{\epsilon^3 M_2}, & \text{when dimension } d=1 \\ \frac{2k}{\pi\epsilon^4 M_3}, & \text{when dimension } d=2, \end{cases} \tag{B.2}$$

with $M_i = \int_0^1 J(r)r^i dr$.

Taylor's series approximation gives:

$$u(y) = u(x) + \nabla u(x)\cdot(y-x) + \frac{1}{2}\nabla^2 u(x) : (y-x)\otimes(y-x) + \frac{1}{6}\nabla^3 u(\xi) : (y-x)\otimes(y-x)\otimes(y-x),$$

where $\xi = \xi(y,x) \in D \cup D_c$. We substitute above in Equation B.1 to get

$$\begin{aligned}
&\mathcal{L}(u)(x) \\
&= c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})\nabla u(x)\cdot(y-x)dy \\
&+ c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})\frac{1}{2}\nabla^2 u(x) : (y-x)\otimes(y-x)dy \\
&+ c\int_{H_\epsilon(x)} J(\frac{|y-x|}{\epsilon})\frac{1}{6}\nabla^3 u(\xi) : (y-x)\otimes(y-x)\otimes(y-x)dy.
\end{aligned}$$

First term in above is zero as J is even function of y and $(y-x)$ is odd function. We consider change in variable $y = x+\epsilon\eta$ where $\eta \in H_1(0)$. Note that $dy = \epsilon^d d\eta$ where d is dimension. We have

$$\begin{aligned}
&\mathcal{L}(u)(x) \\
&= c\int_{H_1(0)} J(|\eta|)\frac{1}{2}\nabla^2 u(x) : \epsilon\eta\otimes\epsilon\eta\epsilon^d d\eta \\
&+ c\int_{H_1(0)} J(|\eta|)\frac{1}{6}\nabla^3 u(\xi) : \epsilon\eta\otimes\epsilon\eta\otimes\epsilon\eta\epsilon^d d\eta \\
&= \frac{c\epsilon^{d+2}}{2}\nabla^2 u(x) : \left[\int_{H_1(0)} J(|\eta|)\eta\otimes\eta d\eta\right] \\
&+ \frac{c\epsilon^{d+3}}{6}\int_{H_1(0)} J(|\eta|)\nabla^3 u(\xi) : \eta\otimes\eta\otimes\eta d\eta.
\end{aligned} \tag{B.3}$$

Assuming u is such that $|\nabla^3 u| < \infty$ at all points, third term is of the order

$$O(c|\nabla^3 u|\epsilon^{d+3})$$

. We analyze the term in square bracket next.

One dimension. When $d = 1$, we have

$$\begin{aligned}&\int_{H_1(0)} J(|\eta|)\eta\otimes\eta d\eta\\ &= \int_{-1}^{1} J(|\eta|)\eta^2 d\eta\\ &= 2\int_0^1 J(r)r^2 dr = 2M_2,\end{aligned} \tag{B.4}$$

where we used the fact that $J(|\eta|)\eta^2$ is even and noted the definition of moment M_2. Substituting this in Equation B.3 and noting the definition of constant c in Equation B.2, we conclude that

$$\mathcal{L}(u)(x) = k\partial_{xx}u(x) + O(|\partial_{xxx}u|\epsilon).$$

Taking $\epsilon \to 0$ gives $\mathcal{L}(u) \to k\partial_{xx}u$.
Two dimension. When $d = 2$, we have

$$\begin{aligned}&\int_{H_1(0)} J(|\eta|)\eta\otimes\eta d\eta\\ &= \int_0^1\int_0^{2\pi} J(|\eta|)\eta\otimes\eta r dr d\theta\\ &= \left(\int_0^1\int_0^{2\pi} J(|\eta|)\eta_i\eta_j r dr d\theta\right) e_i\otimes e_j.\end{aligned}$$

Where e_1, e_2 are basis vector in 2-d, $i, j \in \{1, 2\}$, and Einstein summation is implied above. Note that in cylindrical coordinate, $\eta_1 = r\cos(\theta), \eta_2 = r\sin(\theta)$ and $|\eta| = r$. We use following trigonometric identities

$$\begin{aligned}\int_0^{2\pi} \cos^2(\theta)d\theta &= \pi,\\ \int_0^{2\pi} \sin^2(\theta)d\theta &= \pi,\\ \int_0^{2\pi} \cos(\theta)\sin(\theta)d\theta &= 0\end{aligned} \tag{B.5}$$

to get

$$\int_0^{2\pi} \eta_i\eta_j d\theta = r^2\pi\delta_{ij}$$

where $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ij} = 1$ if $i = j$. Substituting to get

$$\begin{aligned}&\int_{H_1(0)} J(|\eta|)\eta\otimes\eta d\eta\\ &= \left(\int_0^1 J(r)r^3 dr\right)\pi\delta_{ij}e_i\otimes e_j\\ &= \pi M_3\delta_{ij}e_i\otimes e_j,\end{aligned}$$

Substituting this in Equation B.3 and noting the definition of constant c in Equation B.2, we get

$$\begin{aligned}&\mathcal{L}(u)(x)\\ &= \frac{c\epsilon^4}{2}\pi M_3\nabla^2 u(x) : \delta_{ij}e_i\otimes e_j + O(c|\nabla^3 u|\epsilon^5)\\ &= \frac{c\epsilon^4}{2}\pi M_3\nabla\cdot\nabla u(x) + O(c|\nabla^3 u|\epsilon^5),\end{aligned}$$

where we used the fact that

$$\nabla^2 u(x) : \delta_{ij}e_i\otimes e_j = \nabla\cdot\nabla u(x).$$

Substituting definition of c from Equation B.2 to get

$$\mathcal{L}(u)(x) = k\nabla\cdot\nabla u(x) + O(|\nabla^3 u|\epsilon).$$

Taking $\epsilon \to 0$ gives $\mathcal{L}(u) \to k\nabla\cdot\nabla u$.