

ChainQueen: A Real-Time Differentiable Physical Simulator for Soft Robotics (Supplemental Material)

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In this document, we discuss the detailed steps for backward gradient computation in ChainQueen, i.e. the differentiable Moving Least Squares Material Point Method (MLS-MPM) [1]. Again, we summarize the notations in Table I. We assume fixed particle mass m_p , volume V_p^0 , hyperelastic constitutive model (with potential energy ψ_p or Young's modulus E_p and Poisson's ratio ν_p) for simplicity.

TABLE I: List of notations for MLS-MPM.

Symbol	Type	Affiliation	Meaning
Δt	scalar		time step size
Δx	scalar		grid cell size
\mathbf{x}_p	vector	particle	position
V_p^0	scalar	particle	initial volume
\mathbf{v}_p	vector	particle	velocity
\mathbf{C}_p	matrix	particle	affine velocity field [2]
\mathbf{P}_p	matrix	particle	PK1 stress ($\partial\psi_p/\partial\mathbf{F}_p$)
$\boldsymbol{\sigma}_{pa}$	matrix	particle	actuation Cauchy stress
\mathbf{A}_p	matrix	particle	actuation stress (material space)
\mathbf{F}_p	matrix	particle	deformation gradient
\mathbf{x}_i	vector	node	position
m_i	scalar	node	mass
\mathbf{v}_i	vector	node	velocity
\mathbf{p}_i	vector	node	momentum, i.e. $m_i\mathbf{v}_i$
N	scalar		quadratic B-spline function

I. VARIABLE DEPENDENCIES

The MLS-MPM time stepping is defined as follows:

$$\mathbf{P}_p^n = \mathbf{P}_p^n(\mathbf{F}_p^n) + \mathbf{F}_p \boldsymbol{\sigma}_{pa}^n \quad (1)$$

$$m_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) m_p \quad (2)$$

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (3)$$

$$\mathbf{v}_i^n = \frac{1}{m_i^n} \mathbf{p}_i^n \quad (4)$$

$$\mathbf{v}_p^{n+1} = \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n \quad (5)$$

$$\mathbf{C}_p^{n+1} = \frac{4}{\Delta x^2} \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n (\mathbf{x}_i - \mathbf{x}_p^n)^T \quad (6)$$

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \Delta t \mathbf{C}_p^{n+1}) \mathbf{F}_p^n, \quad (7)$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+1} \quad (8)$$

$$(9)$$

* indicates joint second authors.

The forward variable dependency is as follows:

$$\mathbf{x}_p^{n+1} \leftarrow \mathbf{x}_p^n, \mathbf{v}_p^{n+1} \quad (10)$$

$$\mathbf{v}_p^{n+1} \leftarrow \mathbf{x}_p^n, \mathbf{v}_i^n \quad (11)$$

$$\mathbf{C}_p^{n+1} \leftarrow \mathbf{x}_p^n, \mathbf{v}_i^n \quad (12)$$

$$\mathbf{F}_p^{n+1} \leftarrow \mathbf{F}_p^n, \mathbf{C}_p^{n+1} \quad (13)$$

$$\mathbf{p}_i^n \leftarrow \mathbf{x}_p^n, \mathbf{C}_p^n, \mathbf{v}_p^n, \mathbf{P}_p^n, \mathbf{F}_p^n \quad (14)$$

$$\mathbf{v}_i^n \leftarrow \mathbf{p}_i^n, m_i^n \quad (15)$$

$$\mathbf{P}_p^n \leftarrow \mathbf{F}_p^n, \sigma_{pa}^n \quad (16)$$

$$m_i^n \leftarrow \mathbf{x}_p^n \quad (17)$$

$$(18)$$

During back-propagation, we have the following reversed variable dependency:

$$\mathbf{x}_p^{n+1}, \mathbf{v}_p^{n+1}, \mathbf{C}_p^{n+1}, \mathbf{p}_i^{n+1}, m_i \leftarrow \mathbf{x}_p^n \quad (19)$$

$$\mathbf{p}_i^n \leftarrow \mathbf{v}_p^n \quad (20)$$

$$\mathbf{x}_p^{n+1} \leftarrow \mathbf{v}_p^{n+1} \quad (21)$$

$$\mathbf{v}_p^{n+1}, \mathbf{C}_p^{n+1} \leftarrow \mathbf{v}_i^n \quad (22)$$

$$\mathbf{F}_p^{n+1}, \mathbf{P}_p^n, \mathbf{p}_i^n \leftarrow \mathbf{F}_p^n \quad (23)$$

$$\mathbf{F}_p^{n+1} \leftarrow \mathbf{C}_p^{n+1} \quad (24)$$

$$\mathbf{p}_i^n \leftarrow \mathbf{C}_p^n \quad (25)$$

$$\mathbf{v}_i^n \leftarrow \mathbf{p}_i^n \quad (26)$$

$$\mathbf{v}_i^n \leftarrow m_i^n \quad (27)$$

$$\mathbf{p}_i^n \leftarrow \mathbf{P}_p^n \quad (28)$$

$$\mathbf{P}_p^n \leftarrow \sigma_{pa}^n \quad (29)$$

$$(30)$$

We reverse swap two sides of the equations for easier differentiation derivation:

$$\mathbf{x}_p^n \rightarrow \mathbf{x}_p^{n+1}, \mathbf{v}_p^{n+1}, \mathbf{C}_p^{n+1}, \mathbf{p}_i^{n+1}, m_i \quad (31)$$

$$\mathbf{v}_p^n \rightarrow \mathbf{p}_i^n \quad (32)$$

$$\mathbf{v}_p^{n+1} \rightarrow \mathbf{x}_p^{n+1} \quad (33)$$

$$\mathbf{v}_i^n \rightarrow \mathbf{v}_p^{n+1}, \mathbf{C}_p^{n+1} \quad (34)$$

$$\mathbf{F}_p^n \rightarrow \mathbf{F}_p^{n+1}, \mathbf{P}_p^n, \mathbf{p}_i^n \quad (35)$$

$$\mathbf{C}_p^{n+1} \rightarrow \mathbf{F}_p^{n+1} \quad (36)$$

$$\mathbf{C}_p^n \rightarrow \mathbf{p}_i^n \quad (37)$$

$$\mathbf{p}_i^n \rightarrow \mathbf{v}_i^n \quad (38)$$

$$m_i^n \rightarrow \mathbf{v}_i^n \quad (39)$$

$$\mathbf{P}_p^n \rightarrow \mathbf{p}_i^n \quad (40)$$

$$\sigma_{pa}^n \rightarrow \mathbf{P}_p^n \quad (41)$$

$$(42)$$

In the following sections, we derive detailed gradient relationships, in the order of actual gradient computation. The frictional boundary condition gradients are postponed to the end since it is less central, though during computation it belongs to grid operations. Back-propagation in ChainQueen is essentially a reversed process of forward simulation. The computation has three steps, backward particle to grid (P2G), backward grid operations, and backward grid to particle (G2P).

II. BACKWARD PARTICLE TO GRID (P2G)

(A, P2G) For \mathbf{v}_p^{n+1} , we have

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+1} \quad (43)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{v}_{p\alpha}^{n+1}} = \left[\frac{\partial L}{\partial \mathbf{x}_p^{n+1}} \frac{\partial \mathbf{x}_p^{n+1}}{\partial \mathbf{v}_p^{n+1}} \right]_{\alpha} \quad (44)$$

$$= \Delta t \frac{\partial L}{\partial \mathbf{x}_{p\alpha}^{n+1}}. \quad (45)$$

(B, P2G) For \mathbf{C}_p^{n+1} , we have

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \Delta t \mathbf{C}_p^{n+1}) \mathbf{F}_p^n \quad (46)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{C}_{p\alpha\beta}^{n+1}} = \left[\frac{\partial L}{\partial \mathbf{F}_p^{n+1}} \frac{\partial \mathbf{F}_p^{n+1}}{\partial \mathbf{C}_p^{n+1}} \right]_{\alpha\beta} \quad (47)$$

$$= \Delta t \sum_{\gamma} \frac{\partial L}{\partial \mathbf{F}_{p\alpha\gamma}^{n+1}} \mathbf{F}_{p\beta\gamma}^n. \quad (48)$$

Note, the above two gradients should also include the contributions of $\frac{\partial L}{\partial \mathbf{v}_p^n}$ and $\frac{\partial L}{\partial \mathbf{C}_p^n}$ respectively, with n being the next time step.

(C, P2G) For \mathbf{v}_i^n , we have

$$\mathbf{v}_p^{n+1} = \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n \quad (49)$$

$$\mathbf{C}_p^{n+1} = \frac{4}{\Delta x^2} \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n (\mathbf{x}_i - \mathbf{x}_p^n)^T \quad (50)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^n} = \left[\sum_p \frac{\partial L}{\partial \mathbf{v}_p^{n+1}} \frac{\partial \mathbf{v}_p^{n+1}}{\partial \mathbf{v}_i^n} + \sum_p \frac{\partial L}{\partial \mathbf{C}_p^{n+1}} \frac{\partial \mathbf{C}_p^{n+1}}{\partial \mathbf{v}_i^n} \right]_{\alpha} \quad (51)$$

$$= \sum_p \left[\frac{\partial L}{\partial \mathbf{v}_{p\alpha}^{n+1}} N(\mathbf{x}_i - \mathbf{x}_p^n) + \frac{4}{\Delta x^2} N(\mathbf{x}_i - \mathbf{x}_p^n) \sum_{\beta} \frac{\partial L}{\partial \mathbf{C}_{p\alpha\beta}^{n+1}} (\mathbf{x}_{i\beta} - \mathbf{x}_{p\beta}) \right]. \quad (52)$$

III. BACKWARD GRID OPERATIONS

(D, grid) For \mathbf{p}_i^n , we have

$$\mathbf{v}_i^n = \frac{1}{m_i^n} \mathbf{p}_i^n \quad (53)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{p}_{i\alpha}^n} = \left[\frac{\partial L}{\partial \mathbf{v}_i^n} \frac{\partial \mathbf{v}_i^n}{\partial \mathbf{p}_i^n} \right]_{\alpha} \quad (54)$$

$$= \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^n} \frac{1}{m_i^n}. \quad (55)$$

(E, grid) For m_i^n , we have

$$\mathbf{v}_i^n = \frac{1}{m_i^n} \mathbf{p}_i^n \quad (56)$$

$$\Rightarrow \frac{\partial L}{\partial m_i^n} = \frac{\partial L}{\partial \mathbf{v}_i^n} \frac{\partial \mathbf{v}_i^n}{\partial m_i^n} \quad (57)$$

$$= -\frac{1}{(m_i^n)^2} \sum_{\alpha} \mathbf{p}_{i\alpha}^n \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^n} \quad (58)$$

$$= -\frac{1}{m_i^n} \sum_{\alpha} \mathbf{v}_{i\alpha}^n \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^n}. \quad (59)$$

IV. BACKWARD GRID TO PARTICLE (G2P)

(F, G2P) For \mathbf{v}_p^n , we have

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (60)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{v}_{p\alpha}^n} = \left[\sum_i \frac{\partial L}{\partial \mathbf{p}_i^n} \frac{\partial \mathbf{p}_i^n}{\partial \mathbf{v}_p^n} \right]_{\alpha} \quad (61)$$

$$= \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) m_p \frac{\partial L}{\partial \mathbf{p}_{i\alpha}^n}. \quad (62)$$

(G, G2P) For \mathbf{P}_p^n , we have

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (63)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{P}_{p\alpha\beta}^n} = \left[\frac{\partial L}{\partial \mathbf{p}_i^n} \frac{\partial \mathbf{p}_i^n}{\partial \mathbf{P}_p^n} \right]_{\alpha\beta} \quad (64)$$

$$= - \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \frac{4}{\Delta x^2} \Delta t V_p^0 \sum_{\gamma} \frac{\partial L}{\partial \mathbf{p}_{i\alpha}^n} \mathbf{F}_{p\gamma\beta}^n (\mathbf{x}_{i\gamma} - \mathbf{x}_{p\gamma}^n). \quad (65)$$

(H, G2P) For \mathbf{F}_p^n , we have

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \Delta t \mathbf{C}_p^{n+1}) \mathbf{F}_p^n \quad (66)$$

$$\mathbf{P}_p^n = \mathbf{P}_p^n (\mathbf{F}_p^n) + \mathbf{F}_p^n \sigma_{pa}^n \quad (67)$$

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (68)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{F}_{p\alpha\beta}^n} = \left[\frac{\partial L}{\partial \mathbf{F}_p^{n+1}} \frac{\partial \mathbf{F}_p^{n+1}}{\partial \mathbf{F}_p^n} + \frac{\partial L}{\partial \mathbf{P}_p^n} \frac{\partial \mathbf{P}_p^n}{\partial \mathbf{F}_p^n} + \frac{\partial L}{\partial \mathbf{p}_i^n} \frac{\partial \mathbf{p}_i^n}{\partial \mathbf{F}_p^n} \right]_{\alpha\beta} \quad (69)$$

$$= \sum_{\gamma} \frac{\partial L}{\partial \mathbf{F}_{p\gamma\beta}^{n+1}} (\mathbf{I}_{\gamma\alpha} + \Delta t \mathbf{C}_{p\gamma\alpha}^{n+1}) + \sum_{\gamma} \sum_{\eta} \frac{\partial L}{\partial \mathbf{P}_{p\gamma\eta}^n} \frac{\partial^2 \Psi_p}{\partial \mathbf{F}_{p\gamma\eta}^n \partial \mathbf{F}_{p\alpha\beta}^n} + \sum_{\gamma} \frac{\partial L}{\partial \mathbf{P}_{p\alpha\gamma}^n} \sigma_{pa\beta\gamma} \quad (70)$$

$$+ \sum_i -N(\mathbf{x}_i - \mathbf{x}_p^n) \sum_{\gamma} \frac{\partial L}{\partial \mathbf{p}_{i\gamma}^n} \frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_{p\gamma\beta}^n (\mathbf{x}_{i\alpha} - \mathbf{x}_{p\alpha}^n). \quad (71)$$

(I, G2P) For \mathbf{C}_p^n , we have

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (72)$$

$$\Rightarrow \frac{\partial L}{\partial \mathbf{C}_{p\alpha\beta}^n} = \left[\sum_i \frac{\partial L}{\partial \mathbf{p}_i^n} \frac{\partial \mathbf{p}_i^n}{\partial \mathbf{C}_p^n} \right]_{\alpha\beta} \quad (73)$$

$$= \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \frac{\partial L}{\partial \mathbf{p}_{i\alpha}^n} m_p (\mathbf{x}_{i\beta} - \mathbf{x}_{p\beta}^n). \quad (74)$$

(J, G2P) For \mathbf{x}_p^n , we have

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+1} \quad (75)$$

$$\mathbf{v}_p^{n+1} = \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n \quad (76)$$

$$\mathbf{C}_p^{n+1} = \frac{4}{\Delta x^2} \sum_i N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_i^n (\mathbf{x}_i - \mathbf{x}_p^n)^T \quad (77)$$

$$\mathbf{p}_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) \left[m_p \mathbf{v}_p^n + \left(-\frac{4}{\Delta x^2} \Delta t V_p^0 \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) (\mathbf{x}_i - \mathbf{x}_p^n) \right] \quad (78)$$

$$m_i^n = \sum_p N(\mathbf{x}_i - \mathbf{x}_p^n) m_p \quad (79)$$

$$\mathbf{G}_p := \left(-\frac{4}{\Delta x^2} V_p^0 \Delta t \mathbf{P}_p^n \mathbf{F}_p^{nT} + m_p \mathbf{C}_p^n \right) \quad (80)$$

$$\implies \quad (81)$$

$$\frac{\partial L}{\partial \mathbf{x}_{p\alpha}^n} = \left[\frac{\partial L}{\partial \mathbf{x}_p^{n+1}} \frac{\partial \mathbf{x}_p^{n+1}}{\partial \mathbf{x}_p^n} + \frac{\partial L}{\partial \mathbf{v}_p^{n+1}} \frac{\partial \mathbf{v}_p^{n+1}}{\partial \mathbf{x}_p^n} + \frac{\partial L}{\partial \mathbf{C}_p^{n+1}} \frac{\partial \mathbf{C}_p^{n+1}}{\partial \mathbf{x}_p^n} + \frac{\partial L}{\partial \mathbf{p}_i^n} \frac{\partial \mathbf{p}_i^n}{\partial \mathbf{x}_p^n} + \frac{\partial L}{\partial m_i^n} \frac{\partial m_i^n}{\partial \mathbf{x}_p^n} \right]_{\alpha} \quad (82)$$

$$= \frac{\partial L}{\partial \mathbf{x}_{p\alpha}^{n+1}} \quad (83)$$

$$+ \sum_i \sum_{\beta} \frac{\partial L}{\partial \mathbf{v}_{p\beta}^{n+1}} \frac{\partial N(\mathbf{x}_i - \mathbf{x}_p^n)}{\partial \mathbf{x}_{i\alpha}} \mathbf{v}_{i\beta}^n \quad (84)$$

$$+ \sum_i \sum_{\beta} \frac{4}{\Delta x^2} \left\{ -\frac{\partial L}{\partial \mathbf{C}_{p\beta\alpha}^{n+1}} N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{v}_{i\beta} + \sum_{\gamma} \frac{\partial L}{\partial \mathbf{C}_{p\beta\gamma}^{n+1}} \frac{\partial N(\mathbf{x}_i - \mathbf{x}_p^n)}{\partial \mathbf{x}_{i\alpha}} \mathbf{v}_{i\beta} (\mathbf{x}_{i\gamma} - \mathbf{x}_{p\gamma}) \right\} \quad (85)$$

$$+ \sum_i \sum_{\beta} \frac{\partial L}{\partial \mathbf{p}_{i\beta}^n} \left[\frac{\partial N(\mathbf{x}_i - \mathbf{x}_p^n)}{\partial \mathbf{x}_{i\alpha}} (m_p \mathbf{v}_{p\beta}^n + [\mathbf{G}_p(\mathbf{x}_i - \mathbf{x}_p^n)]_{\beta}) - N(\mathbf{x}_i - \mathbf{x}_p^n) \mathbf{G}_{p\beta\alpha} \right] \quad (86)$$

$$+ m_p \sum_i \frac{\partial L}{\partial m_i^n} \frac{\partial N(\mathbf{x}_i - \mathbf{x}_p^n)}{\partial \mathbf{x}_{i\alpha}} \quad (87)$$

$$(88)$$

(K, G2P) For σ_{pa}^n , we have

$$\mathbf{P}_p^n = \mathbf{P}_p^n(\mathbf{F}_p^n) + \mathbf{F}_p \sigma_{pa}^n \quad (89)$$

$$\implies \frac{\partial L}{\partial \sigma_{pa\alpha\beta}^n} = \left[\frac{\partial L}{\partial \mathbf{P}_p^n} \frac{\partial \mathbf{P}_p^n}{\partial \sigma_{pa\alpha\beta}^n} \right]_{\alpha\beta} \quad (90)$$

$$= \sum_{\gamma} \frac{\partial L}{\partial \mathbf{P}_{p\gamma\beta}^{n+1}} \mathbf{F}_{p\gamma\alpha}^n. \quad (91)$$

V. FRICTION PROJECTION GRADIENTS

When there are boundary conditions:

(L, grid) For \mathbf{v}_i^n , we have

$$l_{in} = \sum_{\alpha} \mathbf{v}_{i\alpha} \mathbf{n}_{i\alpha} \quad (92)$$

$$\mathbf{v}_{it} = \mathbf{v}_i - l_{in} \mathbf{n}_i \quad (93)$$

$$l_{it} = \sqrt{\sum_{\alpha} \mathbf{v}_{it\alpha}^2 + \varepsilon} \quad (94)$$

$$\hat{\mathbf{v}}_{it} = \frac{1}{l_{it}} \mathbf{v}_{it} \quad (95)$$

$$l_{it}^* = \max\{l_{it} + c_i \min\{l_{in}, 0\}, 0\} \quad (96)$$

$$\mathbf{v}_i^* = l_{it}^* \hat{\mathbf{v}}_{it} + \max\{l_{in}, 0\} \mathbf{n}_i \quad (97)$$

$$H(x) := [x \geq 0] \quad (98)$$

$$R := l_{it} + c_i \min\{l_{in}, 0\} \quad (99)$$

$$\Rightarrow \frac{\partial L}{\partial l_{it}^*} = \sum_{\alpha} \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^*} \hat{\mathbf{v}}_{it\alpha} \quad (100)$$

$$\frac{\partial L}{\partial \hat{\mathbf{v}}_{it}} = \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^*} l_{it}^* \quad (101)$$

$$\frac{\partial L}{\partial l_{it}} = -\frac{1}{l_{it}^2} \sum_{\alpha} \mathbf{v}_{it\alpha} \frac{\partial L}{\partial \hat{\mathbf{v}}_{it\alpha}} + \frac{\partial L}{\partial l_{it}^*} H(R) \quad (102)$$

$$\frac{\partial L}{\partial \mathbf{v}_{it\alpha}} = \frac{\mathbf{v}_{it\alpha}}{l_{it}} \frac{\partial L}{\partial l_{it}} + \frac{1}{l_{it}} \frac{\partial L}{\partial \hat{\mathbf{v}}_{it\alpha}} \quad (103)$$

$$= \frac{1}{l_{it}} \left[\frac{\partial L}{\partial l_{it}} \mathbf{v}_{it\alpha} + \frac{\partial L}{\partial \hat{\mathbf{v}}_{it\alpha}} \right] \quad (104)$$

$$\frac{\partial L}{\partial l_{in}} = - \left[\sum_{\alpha} \frac{\partial L}{\partial \mathbf{v}_{it\alpha}} \mathbf{n}_{i\alpha} \right] + \frac{\partial L}{\partial l_{it}^*} H(R) c_i H(-l_{in}) + \sum_{\alpha} H(l_{in}) \mathbf{n}_{i\alpha} \frac{\partial L}{\partial \mathbf{v}_{i\alpha}^*} \quad (105)$$

$$\frac{\partial L}{\partial \mathbf{v}_{i\alpha}} = \frac{\partial L}{\partial l_{in}} \mathbf{n}_{i\alpha} + \frac{\partial L}{\partial \mathbf{v}_{it\alpha}} \quad (106)$$

$$(107)$$

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