Hybrid Conjugate Gradient (HCG) Method in Polymer SCFT

Theoretical Notes

February 27, 2026

1 Part I: General Hybrid Conjugate Gradient (HCG) Process

Goal

To construct a robust iterative update scheme for finding the saddle point of a functional $F[\mathbf{\Phi}, \mathbf{\Psi}]$. The functional must be minimized with respect to a set of fields $\mathbf{\Phi}$ and maximized with respect to another set of fields $\mathbf{\Psi}$. Pure Conjugate Gradient (CG) often fails far from the saddle point due to non-convexity, while explicit steepest descent/ascent is unconditionally stable but impractically slow. HCG blends the two to achieve both stability and acceleration.

Setup & Definitions

Vector-valued fields (notation clarification). We treat the unknown fields as *column vectors of scalar component fields*:

$$\mathbf{\Phi}(\mathbf{r}) \equiv \begin{bmatrix} \Phi_1(\mathbf{r}) \\ \vdots \\ \Phi_{n_\Phi}(\mathbf{r}) \end{bmatrix}, \qquad \mathbf{\Psi}(\mathbf{r}) \equiv \begin{bmatrix} \Psi_1(\mathbf{r}) \\ \vdots \\ \Psi_{n_\Psi}(\mathbf{r}) \end{bmatrix}, \tag{1}$$

where *non-bold* symbols like $\Phi_i(\mathbf{r})$ and $\Psi_j(\mathbf{r})$ denote the *components* (elements) of the bold vectors $\mathbf{\Phi}$ and $\mathbf{\Psi}$.

Saddle-point condition. Let the objective functional be $F[\mathbf{\Phi}, \mathbf{\Psi}]$. The physical solution requires:

$$\frac{\delta F}{\delta \mathbf{\Phi}} = \mathbf{0} \quad \text{(Minimum in } \mathbf{\Phi}\text{)}, \qquad \frac{\delta F}{\delta \mathbf{\Psi}} = \mathbf{0} \quad \text{(Maximum in } \mathbf{\Psi}\text{)}. \tag{2}$$

Local functional gradients. At iteration k, define the vector-valued functional gradients by

$$\mathbf{g}_\Phi^{(k)}(\mathbf{r}) \equiv \frac{\delta F}{\delta \mathbf{\Phi}^{(k)}(\mathbf{r})}, \qquad \mathbf{g}_\Psi^{(k)}(\mathbf{r}) \equiv \frac{\delta F}{\delta \mathbf{\Psi}^{(k)}(\mathbf{r})}. \tag{3}$$

Componentwise, this means

$$\left[\mathbf{g}_\Phi^{(k)}(\mathbf{r})\right]_i = \frac{\delta F}{\delta \Phi_i^{(k)}(\mathbf{r})}, \qquad \left[\mathbf{g}_\Psi^{(k)}(\mathbf{r})\right]_j = \frac{\delta F}{\delta \Psi_j^{(k)}(\mathbf{r})}. \tag{4}$$

To handle the saddle point, we assign independent step sizes $\lambda_\Phi > 0$ and $\lambda_\Psi > 0$, and independent hybridization parameters $\alpha_{H,\Phi}, \alpha_{H,\Psi} \in [0, 1]$.

Inner product convention (continuous). For vector-valued fields, the natural L^2 inner product includes a sum over components:

$$\langle \mathbf{a}, \mathbf{b} \rangle \;\equiv\; \sum_{\ell} \int d\mathbf{r}\; a_\ell(\mathbf{r})\, b_\ell(\mathbf{r}), \tag{5}$$

where ℓ runs over the components of the corresponding vector field (e.g., $\ell = 1, \ldots, n_\Phi$ for $\mathbf{g}_\Phi$).

Step-by-step derivation

1. Initialization. At $k = 0$, we have no previous search history. The search directions are initialized along the local gradients. To minimize in $\mathbf{\Phi}$, we descend; to maximize in $\mathbf{\Psi}$, we ascend:

$$\mathbf{d}_\Phi^{(0)}(\mathbf{r}) = -\mathbf{g}_\Phi^{(0)}(\mathbf{r}), \tag{6}$$

$$\mathbf{d}_\Psi^{(0)}(\mathbf{r}) = +\mathbf{g}_\Psi^{(0)}(\mathbf{r}). \tag{7}$$

2. Fletcher–Reeves conjugacy factors (continuous). At step $k+1$, evaluate the new gradients. The Fletcher–Reeves "memory" is the ratio of squared L^2 norms:

$$\gamma_\Phi^{(k+1)} = \frac{\langle \mathbf{g}_\Phi^{(k+1)}, \mathbf{g}_\Phi^{(k+1)} \rangle}{\langle \mathbf{g}_\Phi^{(k)}, \mathbf{g}_\Phi^{(k)} \rangle}, \qquad \gamma_\Psi^{(k+1)} = \frac{\langle \mathbf{g}_\Psi^{(k+1)}, \mathbf{g}_\Psi^{(k+1)} \rangle}{\langle \mathbf{g}_\Psi^{(k)}, \mathbf{g}_\Psi^{(k)} \rangle}. \tag{8}$$

Discrete implementation note (matrix form). In a computer simulation, each (scalar) field is stored on a grid of M points $\{\mathbf{r}_m\}_{m=1}^M$ as a tensor/array. Flatten that array into a vector $\mathbf{g} \in \mathbb{R}^M$ (or $\mathbb{C}^M$), with entries $g_m = g(\mathbf{r}_m)$. For a uniform grid with cell volume ΔV, the integral becomes

$$\int d\mathbf{r}\, g(\mathbf{r})^2 \;\approx\; \Delta V \sum_{m=1}^{M} g_m^2 \;=\; \mathbf{g}^\mathsf{T} (\Delta V\, \mathbf{I})\, \mathbf{g} \;\equiv\; \mathbf{g}^\mathsf{T}\, \mathbf{W}\, \mathbf{g}, \tag{9}$$

where $\mathbf{W} = \Delta V\, \mathbf{I}$ is a diagonal "quadrature weight" matrix. For vector-valued fields (multiple components), stack all components into one long vector (e.g. concatenate component arrays) so the same matrix form applies.

Therefore, the discrete Fletcher–Reeves factors corresponding to Eq. (8) are

$$\gamma_\Phi^{(k+1)} = \frac{\big(\mathbf{g}_\Phi^{(k+1)}\big)^\mathsf{T} \mathbf{W}\, \mathbf{g}_\Phi^{(k+1)}}{\big(\mathbf{g}_\Phi^{(k)}\big)^\mathsf{T} \mathbf{W}\, \mathbf{g}_\Phi^{(k)}}, \qquad \gamma_\Psi^{(k+1)} = \frac{\big(\mathbf{g}_\Psi^{(k+1)}\big)^\mathsf{T} \mathbf{W}\, \mathbf{g}_\Psi^{(k+1)}}{\big(\mathbf{g}_\Psi^{(k)}\big)^\mathsf{T} \mathbf{W}\, \mathbf{g}_\Psi^{(k)}}. \tag{10}$$

On a uniform grid, the common factor ΔV cancels between numerator and denominator, so many codes simply compute "sum of squares":

$$\gamma_\Phi^{(k+1)} = \frac{\|\mathbf{g}_\Phi^{(k+1)}\|_2^2}{\|\mathbf{g}_\Phi^{(k)}\|_2^2}, \qquad \gamma_\Psi^{(k+1)} = \frac{\|\mathbf{g}_\Psi^{(k+1)}\|_2^2}{\|\mathbf{g}_\Psi^{(k)}\|_2^2}. \tag{11}$$

3. Hybrid search direction construction. We linearly combine the strict steepest descent/ascent direction with the previous search direction, damped by α_H:

$$\mathbf{d}_\Phi^{(k+1)}(\mathbf{r}) = -\mathbf{g}_\Phi^{(k+1)}(\mathbf{r}) + \alpha_{H,\Phi}\, \gamma_\Phi^{(k+1)}\, \mathbf{d}_\Phi^{(k)}(\mathbf{r}), \tag{12}$$

$$\mathbf{d}_\Psi^{(k+1)}(\mathbf{r}) = +\mathbf{g}_\Psi^{(k+1)}(\mathbf{r}) + \alpha_{H,\Psi}\, \gamma_\Psi^{(k+1)}\, \mathbf{d}_\Psi^{(k)}(\mathbf{r}). \tag{13}$$

Note: If $\alpha_H \to 0$, Eqs. (12)–(13) reduce to explicit steepest descent/ascent. If $\alpha_H \to 1$, we recover pure Fletcher–Reeves CG.

4. Field update. The fields are updated along the established search directions:

$$\mathbf{\Phi}^{(k+1)}(\mathbf{r}) = \mathbf{\Phi}^{(k)}(\mathbf{r}) + \lambda_\Phi \, \mathbf{d}_\Phi^{(k+1)}(\mathbf{r}), \tag{14}$$

$$\mathbf{\Psi}^{(k+1)}(\mathbf{r}) = \mathbf{\Psi}^{(k)}(\mathbf{r}) + \lambda_\Psi \, \mathbf{d}_\Psi^{(k+1)}(\mathbf{r}). \tag{15}$$

2 Part II: Example - Incompressible AB Diblock Copolymer Melt

Goal

Apply the HCG formalism explicitly to a standard continuous Gaussian linear AB diblock copolymer melt, evaluating the functional gradients and structuring the specific update loop for the pressure field $\mu_+(\mathbf{r})$ and exchange field $\mu_-(\mathbf{r})$.

Setup & Definitions

Following standard conventions, we express the intensive free energy functional per chain in units of k_BT, $F[\mu_+, \mu_-] \equiv \beta H/n$:

$$F[\mu_+, \mu_-] = \frac{1}{V} \int d\mathbf{r} \left[-\mu_+(\mathbf{r}) + \frac{1}{\chi_{AB} N} \, \mu_-(\mathbf{r})^2 \right] - \ln Q[\mu_+, \mu_-]. \tag{16}$$

Here μ_+ and μ_- are the sum and difference auxiliary fields, respectively; χ_{AB} is the Flory–Huggins parameter and N is the degree of polymerization. Q is the single-chain partition function.

The thermodynamic saddle point dictates that F must be **minimized** with respect to the exchange field μ_- and **maximized** with respect to the pressure field μ_+.

Step-by-step derivation

1. Evaluate functional gradients. Taking functional derivatives yields the local constraints. At iteration k:

$$g_+^{(k)}(\mathbf{r}) \equiv \frac{\delta F}{\delta \mu_+^{(k)}(\mathbf{r})} = \phi_A^{(k)}(\mathbf{r}) + \phi_B^{(k)}(\mathbf{r}) - 1, \tag{17}$$

$$g_-^{(k)}(\mathbf{r}) \equiv \frac{\delta F}{\delta \mu_-^{(k)}(\mathbf{r})} = \frac{2\mu_-^{(k)}(\mathbf{r})}{\chi_{AB} N} - \left[\phi_A^{(k)}(\mathbf{r}) - \phi_B^{(k)}(\mathbf{r}) \right]. \tag{18}$$

Here, $\phi_A^{(k)}$ and $\phi_B^{(k)}$ are the segment volume fractions computed by solving the modified diffusion equations with fields $\mu_+^{(k)}, \mu_-^{(k)}$.

2. Compute the conjugacy factors. Using the continuous L^2 norm,

$$\gamma_+^{(k)} = \frac{\int d\mathbf{r} \left(g_+^{(k)}(\mathbf{r}) \right)^2}{\int d\mathbf{r} \left(g_+^{(k-1)}(\mathbf{r}) \right)^2}, \qquad \gamma_-^{(k)} = \frac{\int d\mathbf{r} \left(g_-^{(k)}(\mathbf{r}) \right)^2}{\int d\mathbf{r} \left(g_-^{(k-1)}(\mathbf{r}) \right)^2}. \tag{19}$$

(For $k = 0$, simply set $\gamma_+^{(0)} = \gamma_-^{(0)} = 0$.)

Discrete form (AB melt). If $g_\pm(\mathbf{r})$ are stored on a grid and flattened into vectors $\mathbf{g}_\pm \in \mathbb{R}^M$, then Eq. (19) is implemented as

$$\gamma_+^{(k)} = \frac{\left(\mathbf{g}_+^{(k)}\right)^{\mathsf{T}} \mathbf{W}\, \mathbf{g}_+^{(k)}}{\left(\mathbf{g}_+^{(k-1)}\right)^{\mathsf{T}} \mathbf{W}\, \mathbf{g}_+^{(k-1)}}, \qquad \gamma_-^{(k)} = \frac{\left(\mathbf{g}_-^{(k)}\right)^{\mathsf{T}} \mathbf{W}\, \mathbf{g}_-^{(k)}}{\left(\mathbf{g}_-^{(k-1)}\right)^{\mathsf{T}} \mathbf{W}\, \mathbf{g}_-^{(k-1)}}, \tag{20}$$

with $\mathbf{W} = \Delta V\, \mathbf{I}$ for a uniform grid (often ΔV cancels).

3. Determine search directions. Mapping $\mu_+ \to$ "ascend" and $\mu_- \to$ "descend", we construct:

$$d_+^{(k)}(\mathbf{r}) = +g_+^{(k)}(\mathbf{r}) + \alpha_{H,+}\, \gamma_+^{(k)}\, d_+^{(k-1)}(\mathbf{r}), \tag{21}$$

$$d_-^{(k)}(\mathbf{r}) = -g_-^{(k)}(\mathbf{r}) + \alpha_{H,-}\, \gamma_-^{(k)}\, d_-^{(k-1)}(\mathbf{r}). \tag{22}$$

Notice the critical sign difference: $+g_+$ points *up* the gradient to enforce $\phi_A + \phi_B = 1$, whereas $-g_-$ points *down* the gradient to minimize the exchange energy.

Final result & structure

Complete HCG Update Scheme for AB Melt

Given fields at step k, the fields for step $k+1$ are obtained via:

$$\mu_+^{(k+1)}(\mathbf{r}) = \mu_+^{(k)}(\mathbf{r}) + \lambda_+ \Big[+ g_+^{(k)}(\mathbf{r}) + \alpha_{H,+}\, \gamma_+^{(k)}\, d_+^{(k-1)}(\mathbf{r}) \Big], \tag{23}$$

$$\mu_-^{(k+1)}(\mathbf{r}) = \mu_-^{(k)}(\mathbf{r}) + \lambda_- \Big[- g_-^{(k)}(\mathbf{r}) + \alpha_{H,-}\, \gamma_-^{(k)}\, d_-^{(k-1)}(\mathbf{r}) \Big]. \tag{24}$$

Implementation Notes:

- **Damping (α_H):** Usually, $\alpha_{H,+} \approx \alpha_{H,-} \approx 0.1 \sim 0.4$. If the SCFT loop exhibits oscillatory behavior, lower α_H toward 0 to damp the "momentum" and recover the more stable steepest-descent/ascent behavior.