Further Development of the Diagonalization Algorithm for Multidimensional Diffusion

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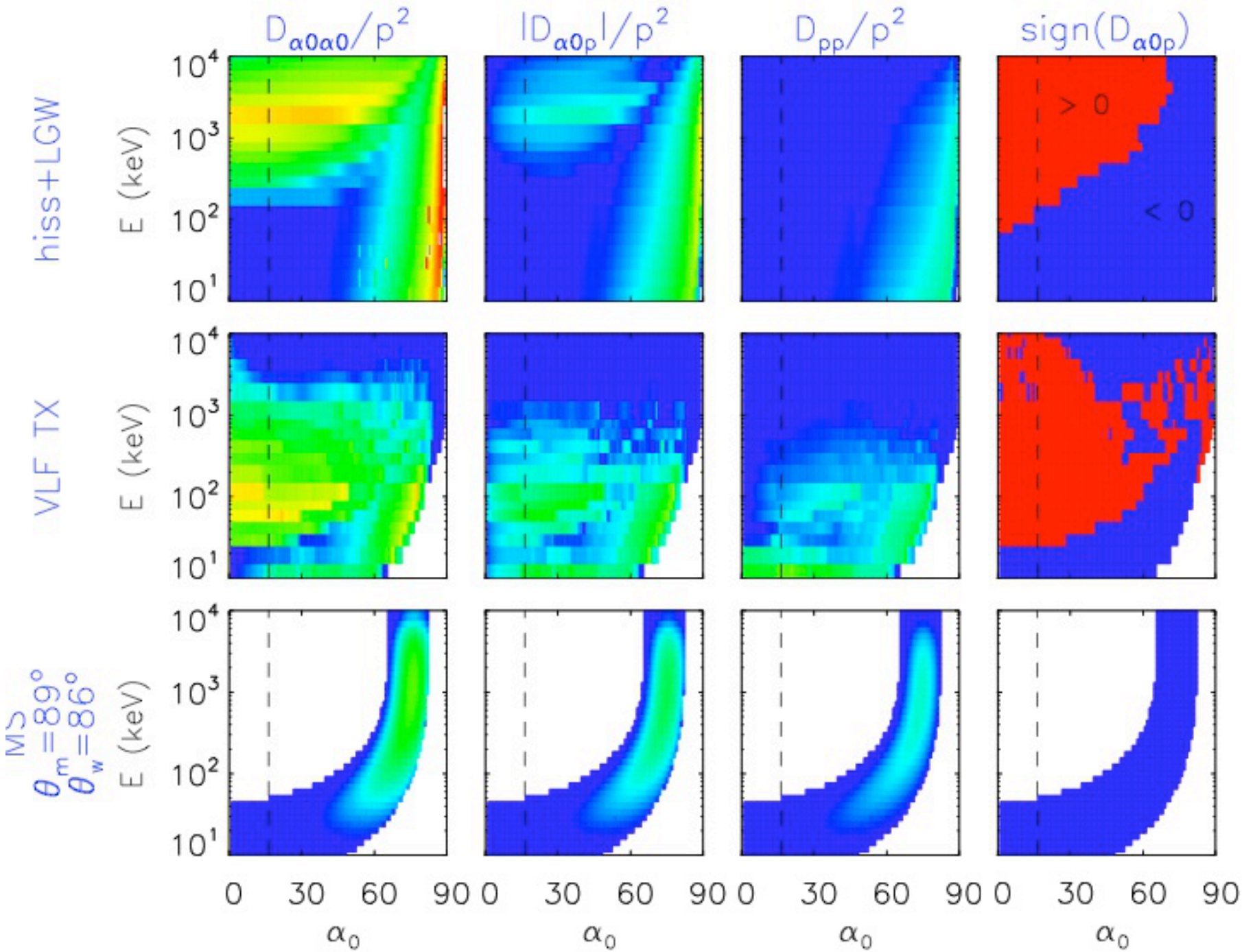
Wave-particle interactions are usually described by a multidimensional diffusion equation. Waves include chorus, hiss, EMIC, MS waves. Cyclotron-resonant quasi-linear theory are most common, but bounce resonance and non-resonant interactions can also be formulated this way.

Including cross diffusion ($D_{\alpha_0 p}$) is now standard practice.

Several approaches work reasonably well, including FI and ADI (traditional, grid-based), SDE (particle) and layer methods (grid-based, but SDE-like), and diagonalization (grid-based).

When $D_{\alpha_0 p} \neq 0$, the traditional grid-based methods don't guarantee good behavior ($f > 0$) for arbitrary (discontinuous) ICs, BCs, D, even if formally linearly stable.



Albert et al., Quasi-linear simulations of inner radiation belt electron pitch angle and energy distributions, Geophys. Res. Lett., 43, doi:10.1002/2016GL067938.

Other people are also still wrestling with this:

"The upper energy boundary (10 MeV) can be set to zero, because the flux at this energy is very low. However, we found that the simulation maintains a very low value of PSD at the upper boundary and is more stable when we set up the derivative with respect to energy to zero, instead of setting up the value of PSD to zero at this boundary"
– Drozdov, et al. (2015), Energetic, relativistic, and ultrarelativistic electrons: Comparison of long-term VERB code simulations with Van Allen Probes measurements, JGR, doi:10.1002/2014JA020637.

"Recently, Subbotin and Shprits [2012] suggested performing 3-D simulations on one grid of modified adiabatic invariants. This approach allows the elimination of interpolation between the numerical grids which can either lead to numerical errors or, in the case of accurate spline interpolation, cause unstable behavior of the code"
– Shprits, et al. (2015), Combined convective and diffusive simulations: VERB-4D comparison with 17 March 2013 Van Allen Probes observations, GRL, doi:10.1002/2015GL065230.

The 2D diffusion equation is

$$\frac{\partial f}{\partial t} = \frac{1}{J}\Big[\frac{\partial}{\partial \alpha_0} J\Big(D_{\alpha_0\alpha_0}\frac{\partial f}{\partial \alpha_0} + D_{\alpha_0 p}\frac{\partial f}{\partial p}\Big) + \frac{\partial}{\partial p} J\Big(D_{\alpha_0 p}\frac{\partial f}{\partial \alpha_0} + D_{pp}\frac{\partial f}{\partial p}\Big)\Big],$$

where $J = \Big|\frac{\partial(J_1, J_2)}{\partial(\alpha_0, p)}\Big|$, and in this notation $D_{\alpha_0\alpha_0} \sim (\Delta\alpha_0)^2/\Delta t$,

$D_{\alpha_0 p} \sim (\Delta\alpha_0 \Delta p)/\Delta t$, $D_{pp} \sim (\Delta p)^2/\Delta t$.

Going from (α_0, p) to any (Q_1, Q_2) gives

$$\begin{bmatrix} \tilde{D}_{11} & \tilde{D}_{12} \\ \tilde{D}_{12} & \tilde{D}_{22} \end{bmatrix} = \begin{bmatrix} \frac{\partial Q_1}{\partial \alpha_0} & \frac{\partial Q_1}{\partial p} \\ \frac{\partial Q_2}{\partial \alpha_0} & \frac{\partial Q_2}{\partial p} \end{bmatrix} \begin{bmatrix} D_{\alpha_0\alpha_0} & D_{\alpha_0 p} \\ D_{\alpha_0 p} & D_{pp} \end{bmatrix} \begin{bmatrix} \frac{\partial Q_1}{\partial \alpha_0} & \frac{\partial Q_2}{\partial \alpha_0} \\ \frac{\partial Q_1}{\partial p} & \frac{\partial Q_2}{\partial p} \end{bmatrix}.$$

We want $\tilde{D}_{12} = 0$.

Simplest possible finite difference scheme:

$$\frac{f_{ij}^{n+1} - f_{ij}^{n}}{\Delta t} = \left\{ D^{11}_{i+\frac{1}{2}j} \frac{f_{i+1j}^{n} - f_{ij}^{n}}{\Delta J_1} - D^{11}_{i-\frac{1}{2}j} \frac{f_{ij}^{n} - f_{i-1j}^{n}}{\Delta J_1} \right\} \Big/ \Delta J_1$$

$$+ \left\{ D^{12}_{i+1j} \frac{f_{i+1j+1}^{n} - f_{i+1j-1}^{n}}{2\Delta J_2} - D^{12}_{i-1j} \frac{f_{i-1j+1}^{n} - f_{i-1j-1}^{n}}{2\Delta J_2} \right\} \Big/ 2\Delta J_1$$

$$+ \left\{ D^{12}_{ij+1} \frac{f_{i+1j+1}^{n} - f_{i-1j+1}^{n}}{2\Delta J_1} - D^{12}_{ij-1} \frac{f_{i+1j-1}^{n} - f_{i-1j-1}^{n}}{2\Delta J_1} \right\} \Big/ 2\Delta J_2$$

$$+ \left\{ D^{22}_{ij+\frac{1}{2}} \frac{f_{ij+1}^{n} - f_{ij}^{n}}{\Delta J_2} - D^{22}_{ij-\frac{1}{2}} \frac{f_{ij}^{n} - f_{ij-1}^{n}}{\Delta J_2} \right\} \Big/ \Delta J_2,$$

or

$$f_{ij}^{n+1} =$$

$$\frac{D^{11}_{i+\frac{1}{2}j}\Delta t}{\Delta J_1^2} f^n_{i+1j} + \frac{D^{11}_{i-\frac{1}{2}j}\Delta t}{\Delta J_1^2} f^n_{i-1j} + \frac{D^{22}_{ij-\frac{1}{2}}\Delta t}{\Delta J_2^2} f^n_{ij-1} + \frac{D^{22}_{ij+\frac{1}{2}}\Delta t}{\Delta J_2^2} f^n_{ij+1}$$

$$+\left\{1 - \left(\frac{D^{11}_{i+\frac{1}{2}j}\Delta t}{\Delta J_1^2} + \frac{D^{11}_{i-\frac{1}{2}j}\Delta t}{\Delta J_1^2} + \frac{D^{22}_{ij-\frac{1}{2}}\Delta t}{\Delta J_2^2} + \frac{D^{22}_{ij+\frac{1}{2}}\Delta t}{\Delta J_2^2}\right)\right\} f^n_{ij}$$

$$+\frac{(D^{12}_{i+1j}+D^{12}_{ij+1})\Delta t}{4\Delta J_1 \Delta J_2} f^n_{i+1j+1} - \frac{(D^{12}_{i+1j}+D^{12}_{ij-1})\Delta t}{4\Delta J_1 \Delta J_2} f^n_{i+1j-1}$$

$$-\frac{(D^{12}_{i-1j}+D^{12}_{ij+1})\Delta t}{4\Delta J_1 \Delta J_2} f^n_{i-1j+1} + \frac{(D^{12}_{i-1j}+D^{12}_{ij-1})\Delta t}{4\Delta J_1 \Delta J_2} f^n_{j-1j-1}.$$

Because of the cross terms, no $\Delta t > 0$ can guarantee $f_{ij}^{n+1} > 0$.

Solution: change variables, make the cross terms vanish.

Choosing $Q_1 = \alpha_0$ leads to $\left.\dfrac{dp}{d\alpha_0}\right|_{Q_2} = \dfrac{D_{\alpha_0 p}}{D_{\alpha_0\alpha_0}}$

and $\tilde{D}_{11} = D_{\alpha_0\alpha_0}, \quad \tilde{D}_{22} = \left(\dfrac{\partial Q_2}{\partial p}\right)^2 \left(D_{pp} - \dfrac{D^2_{\alpha_0 p}}{D_{\alpha_0\alpha_0}}\right).$

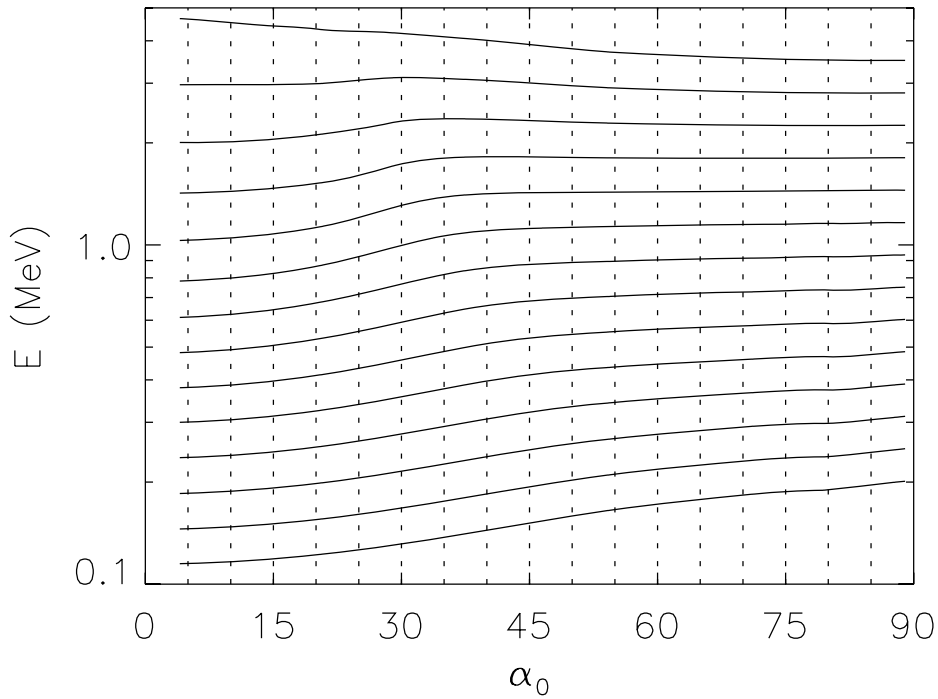
Then, $\dfrac{\partial f}{\partial t} = \dfrac{1}{G}\left(\dfrac{\partial}{\partial Q_1} G\tilde{D}_{11}\dfrac{\partial f}{\partial Q_1} + \dfrac{\partial}{\partial Q_2} G\tilde{D}_{22}\dfrac{\partial f}{\partial Q_2}\right), \quad G = \left|\dfrac{\partial(J_1, J_2)}{\partial(Q_1, Q_2)}\right|,$

(This was done in Albert and Young, GRL 2005.)

This equation is much better-behaved numerically.

[In all of this, can replace (α_0, p) with $(\sin\alpha_0, \log p)$ or $(\cos\alpha_0, \log E)$, etc.]

In the (α_0, p) plane, constant-Q_1 curves are vertical and constant-Q_2 curves have slope $D_{\alpha_0 p}/D_{\alpha_0\alpha_0}$, which is typically small.



But if $D_{pp} > |D_{\alpha_0 p}| > D_{\alpha_0\alpha_0}$ (which can happen at large E), better to take $Q_1 = p$, which leads to $\left.\dfrac{dp}{d\alpha_0}\right|_{Q_2} = \dfrac{D_{\alpha_0 p}}{D_{pp}}$ and

$$\tilde{D}_{11} = D_{pp}, \quad \tilde{D}_{22} = \left(\frac{\partial Q_2}{\partial \alpha_0}\right)^2 \left(D_{\alpha_0\alpha_0} - \frac{D^2_{\alpha_0 p}}{D_{pp}}\right).$$

More generally, choose $\left.\frac{dp}{d\alpha_0}\right|_{Q_1} = \frac{W_2}{W_1}$, $\left.\frac{dp}{d\alpha_0}\right|_{Q_2} = \frac{V_2}{V_1}$, where

$\begin{bmatrix} V_1 \\ V_2 \end{bmatrix}$ and $\begin{bmatrix} W_1 \\ W_2 \end{bmatrix}$ are the E.V.s of $\begin{bmatrix} D_{\alpha_0\alpha_0} & D_{\alpha_0 p} \\ D_{\alpha_0 p} & D_{pp} \end{bmatrix}$, with e.v.s $\lambda_\pm$.

This also leads to $\tilde{D}_{12} = 0$, and

$$\tilde{D}_{11} = \lambda_+ \Big[\Big(\frac{\partial Q_1}{\partial \alpha_0} \Big)^2 + \Big(\frac{\partial Q_1}{\partial p} \Big)^2 \Big],$$

$$\tilde{D}_{22} = \lambda_- \Big[\Big(\frac{\partial Q_2}{\partial \alpha_0} \Big)^2 + \Big(\frac{\partial Q_2}{\partial p} \Big)^2 \Big].$$

Lots of nice properties, e.g., Q-curves are orthogonal, and

$$\tilde{D}_{11} \geq \max[D_{\alpha_0,\alpha_0}, D_{pp}] \geq \min[D_{\alpha_0,\alpha_0}, D_{pp}] \geq \tilde{D}_{22} \geq 0.$$

Also, generalizes to 3D.

Using bilinear interpolation of a table of D values,

$$\left.\frac{dp}{d\alpha_0}\right|_{Q_2} = -\left.\frac{d\alpha_0}{dp}\right|_{Q_1} \approx A + B\alpha_0 + Cp + F\alpha_0 p,$$

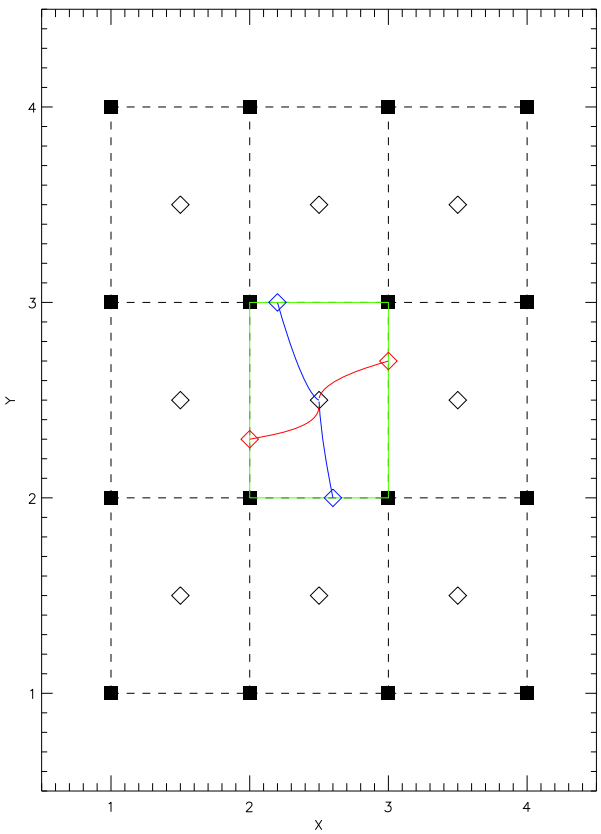
yields closed form expressions for Q_1 and Q_2:

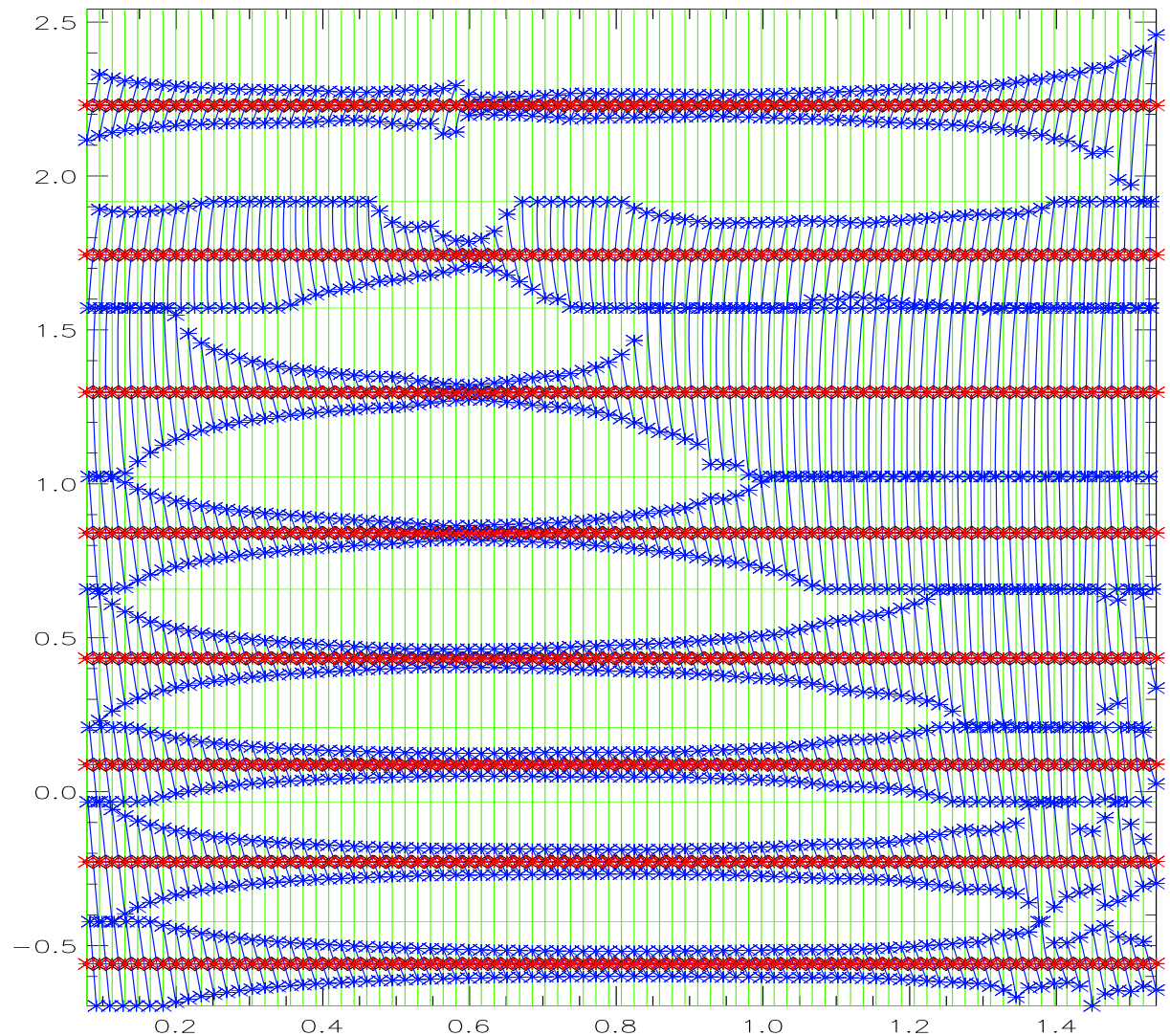
$$Q_1(\alpha_0, p) = \quad \alpha_0 e^{[Bp+Fp^2/2]} + \int_0^p dp'(A + Cp')e^{[Bp'+Fp'^2/2]},$$

$$Q_2(\alpha_0, p) = \quad pe^{-[C\alpha_0+F\alpha_0^2/2]} - \int_0^{\alpha_0} d\alpha'(A + B\alpha')e^{-[C\alpha'+F\alpha'^2/2]},$$

constructed separately in each cell.
(Can write the integrals in terms of the error function, and so on.)

This then gives $\dfrac{\partial Q_1}{\partial \alpha_0}$, etc.

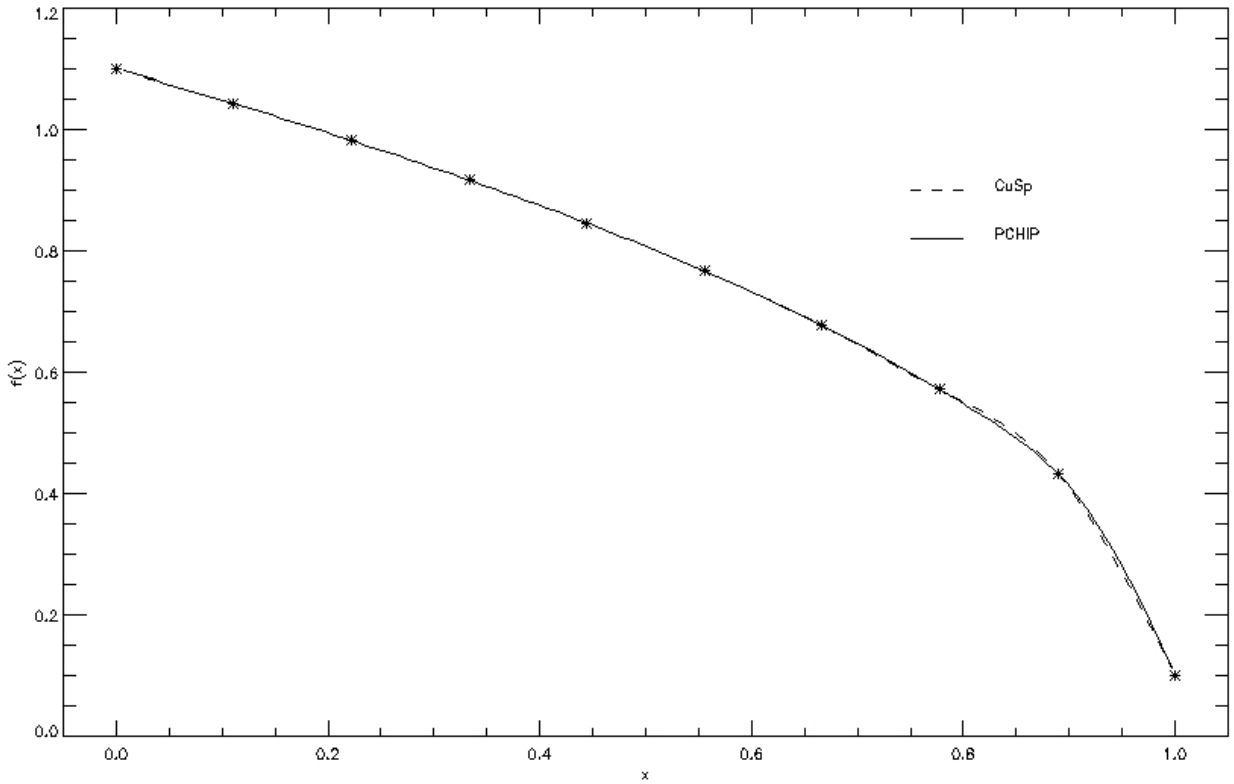




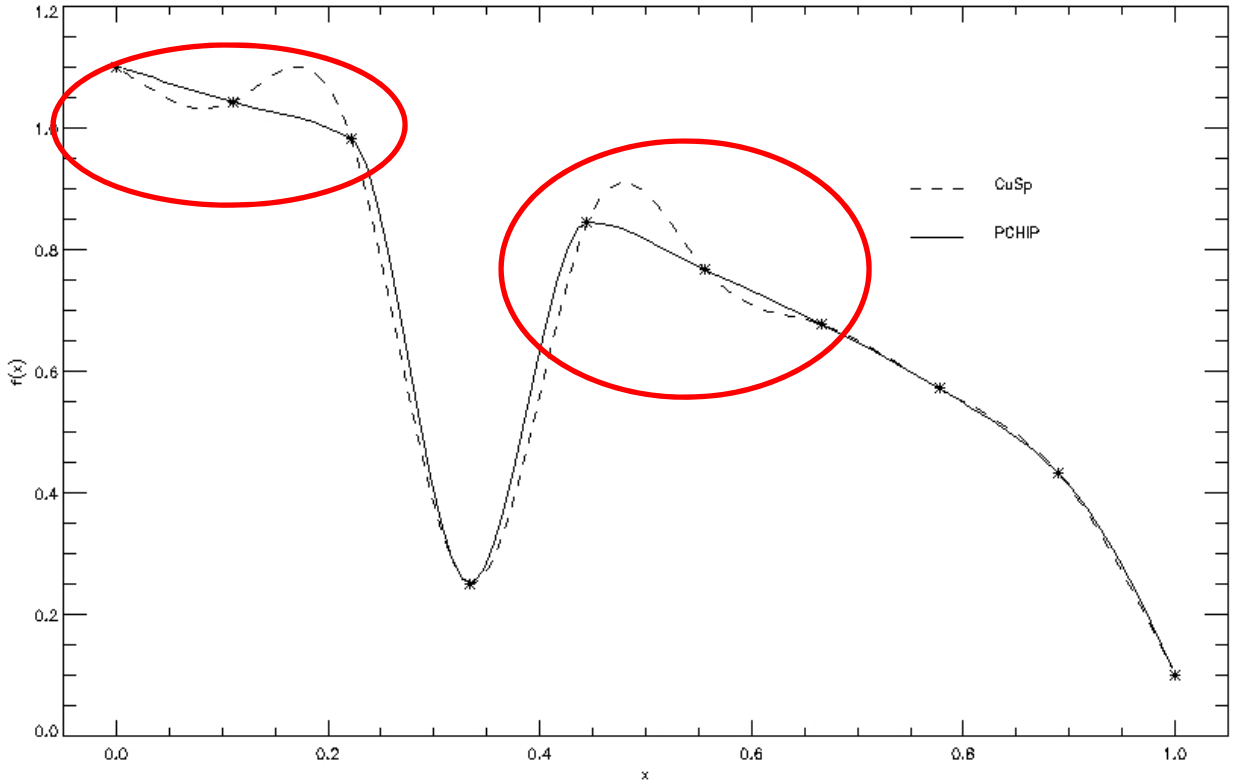
- Trace the constant-Q curves to cell edges (only has to be done once)
- Interpolate f at edges
- Update f with finite differences in (Q_1, Q_2)

To get f at cell edges, want something better than linear interpolation.

For monotonic data, cubic splines work well. Another good choice is piecewise-continuous Hermite interpolating polynomials (PCHIP):



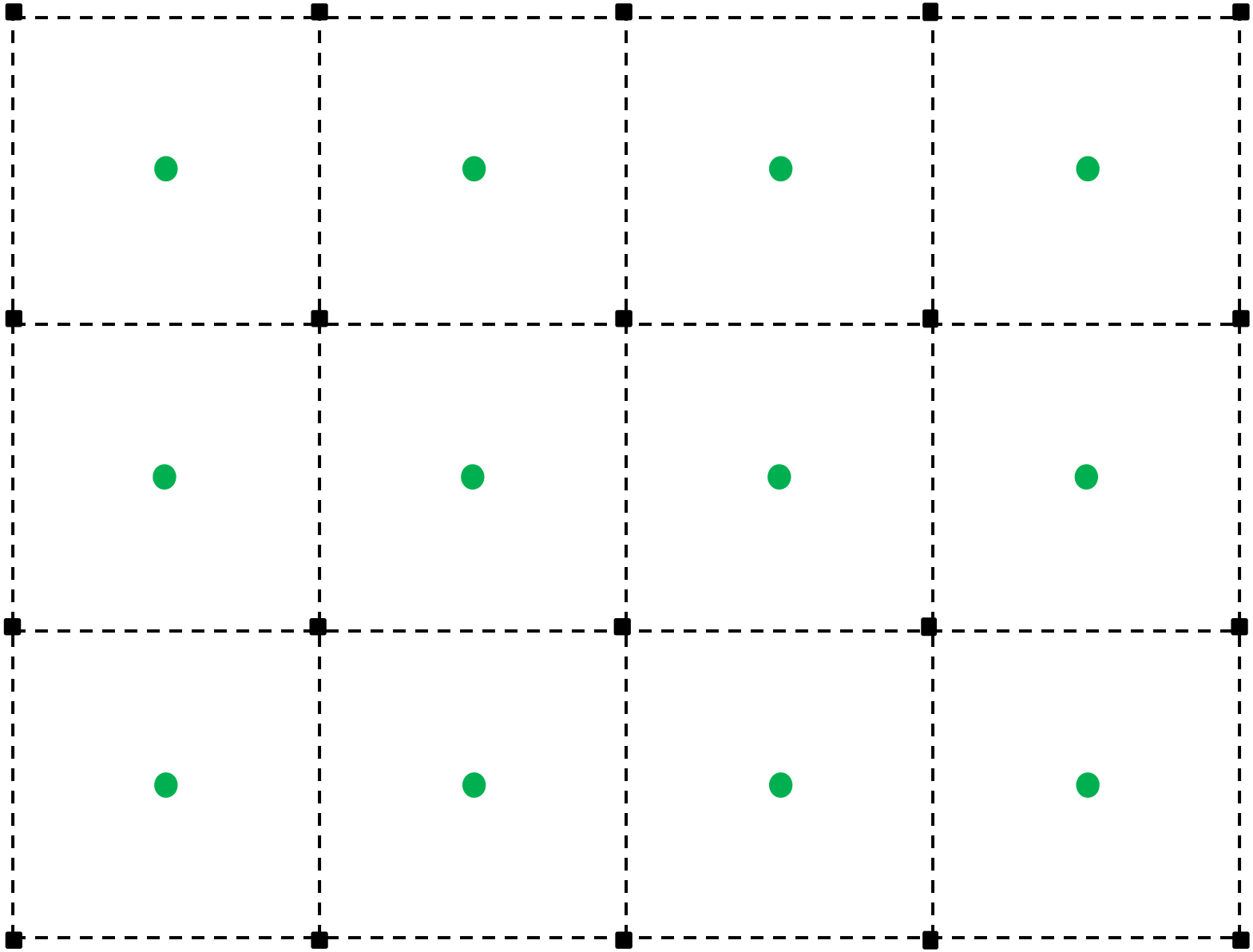
For non-monotonic data, splines can have oscillations. PCHIP doesn't.



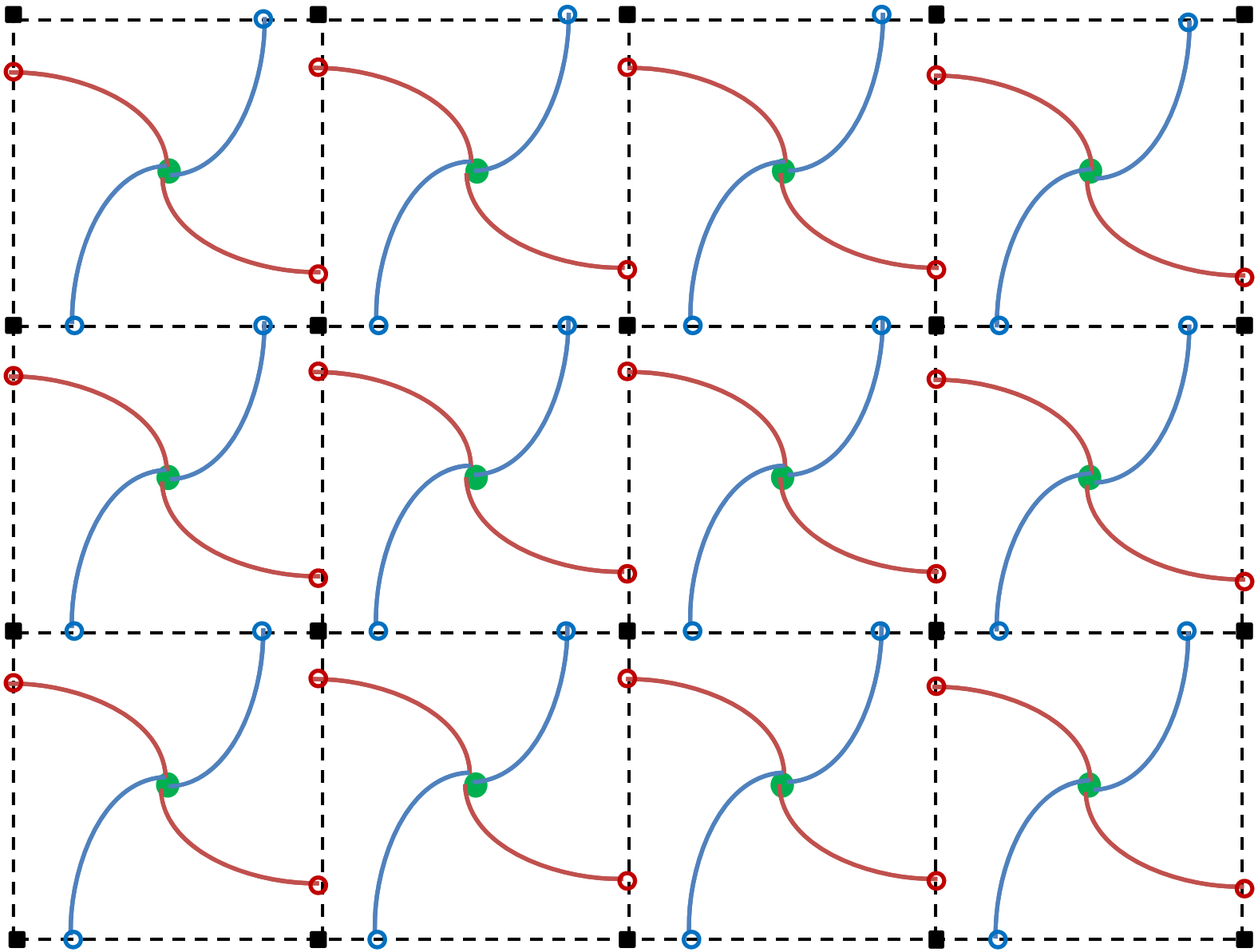
For even better schemes, see Tao, X., L. Zhang, C. Wang, X. Li, J. M. Albert, and A. A. Chan (2016), An efficient and positivity-preserving layer method for modeling radiation belt diffusion processes, *J. Geophys. Res. Space Physics*, *121*, 305–320, doi:10.1002/2015JA022064.

For either, using 1D interpolants on a 2D staggered grid is slightly involved:

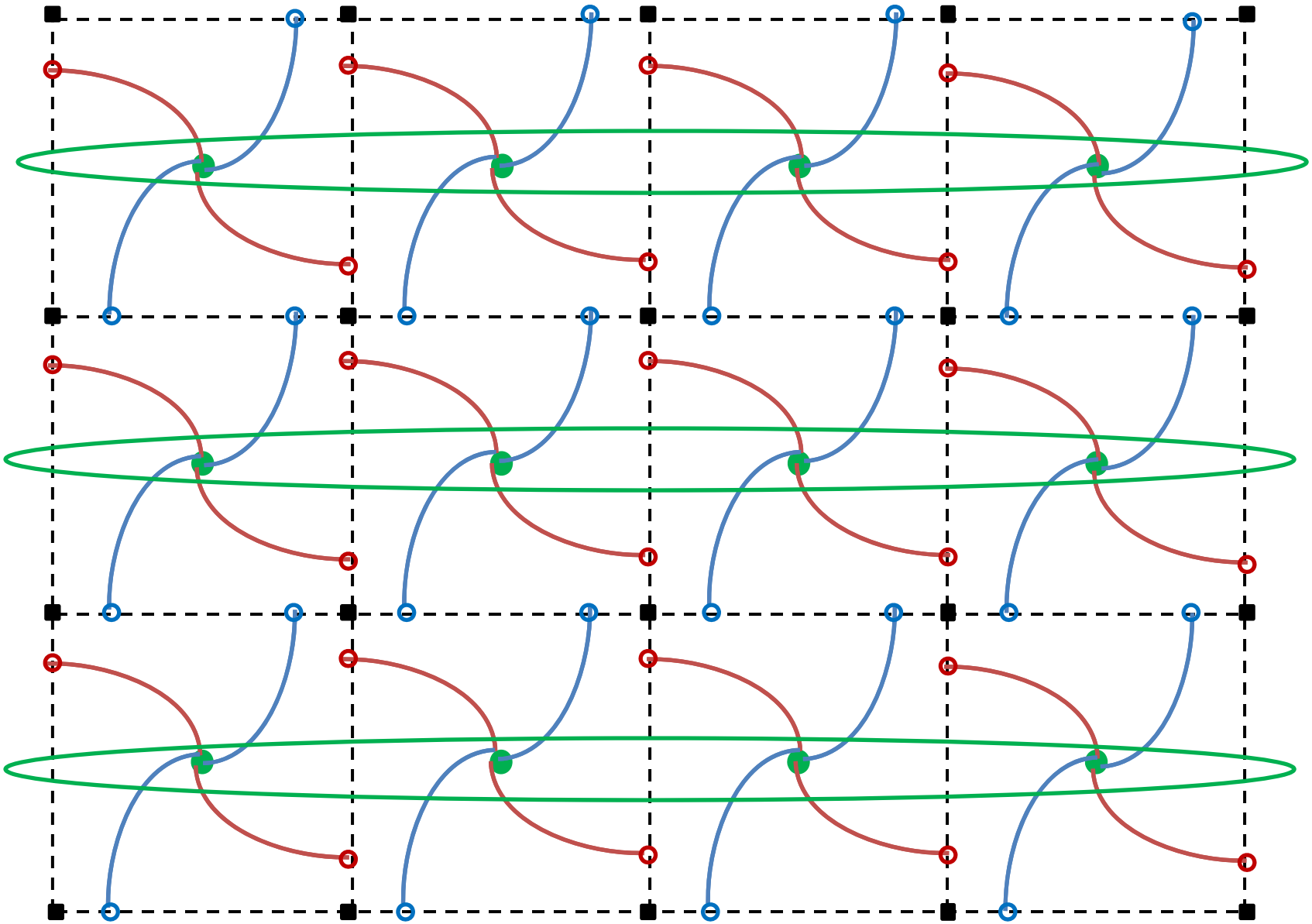
Staggered grid: D ■ f ●



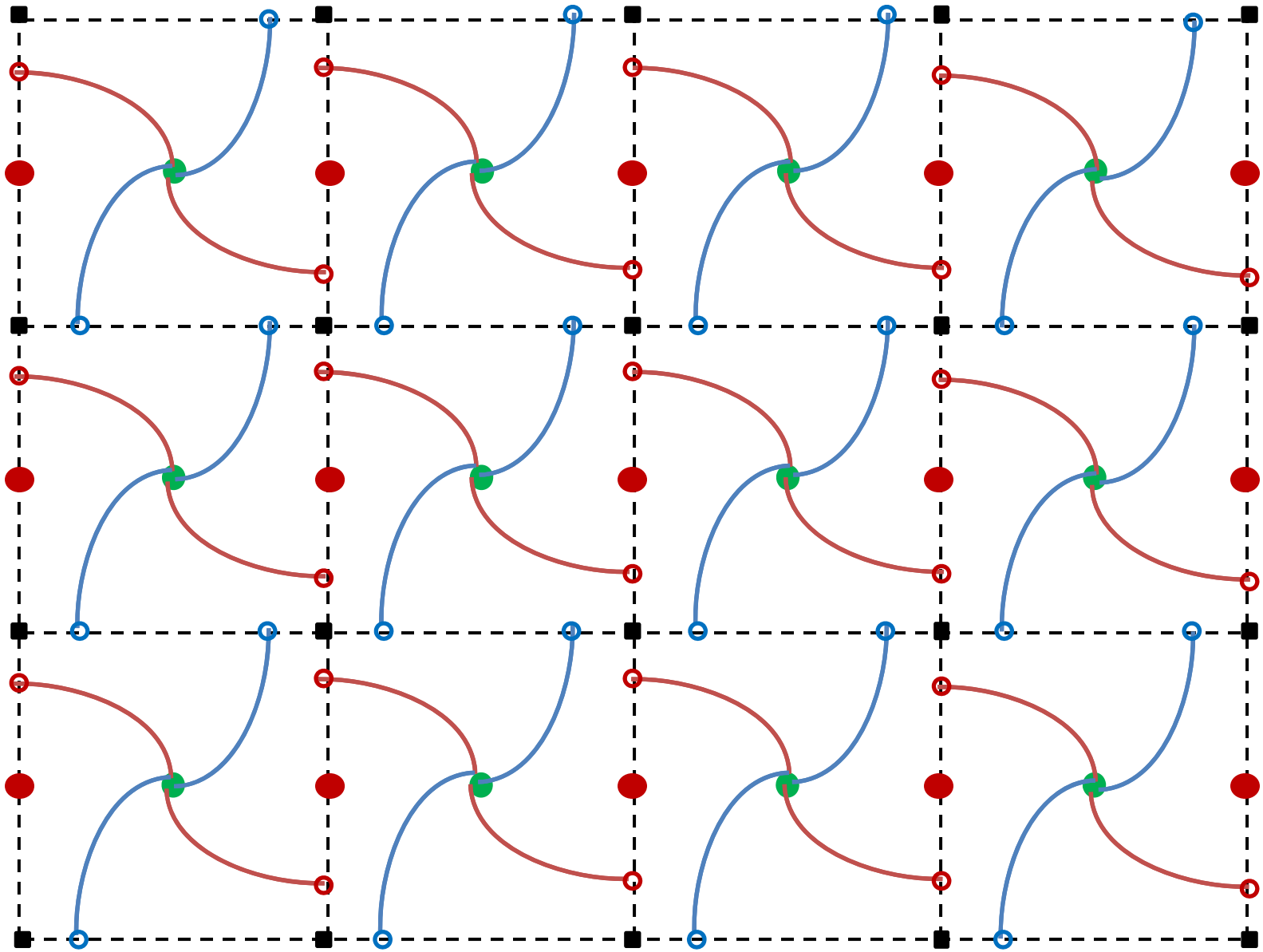
Trace Q_1=c and Q_2=c to cell edges: will need f there.



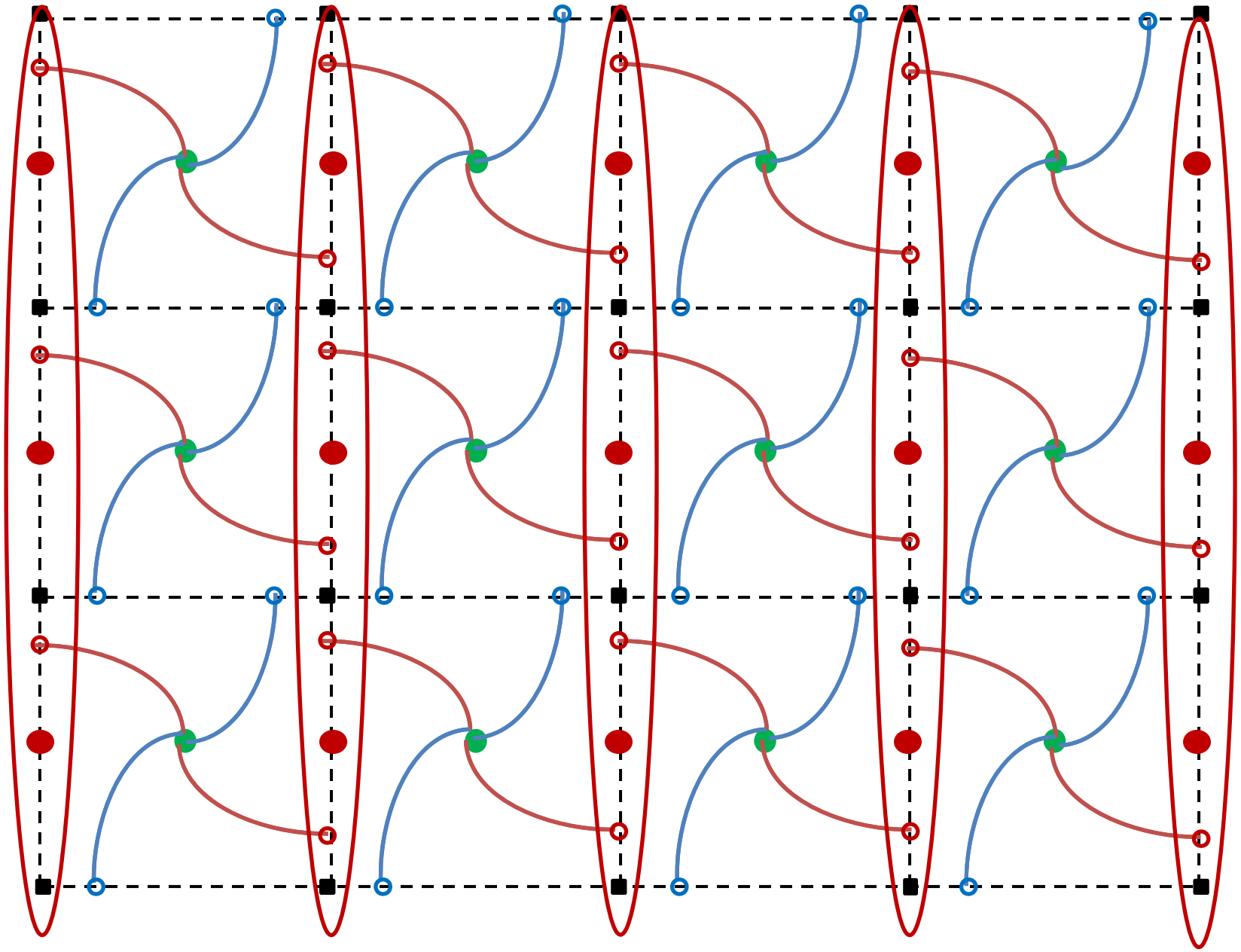
Step 1a: Interpolate f this way … (splines, PCHIP, …)



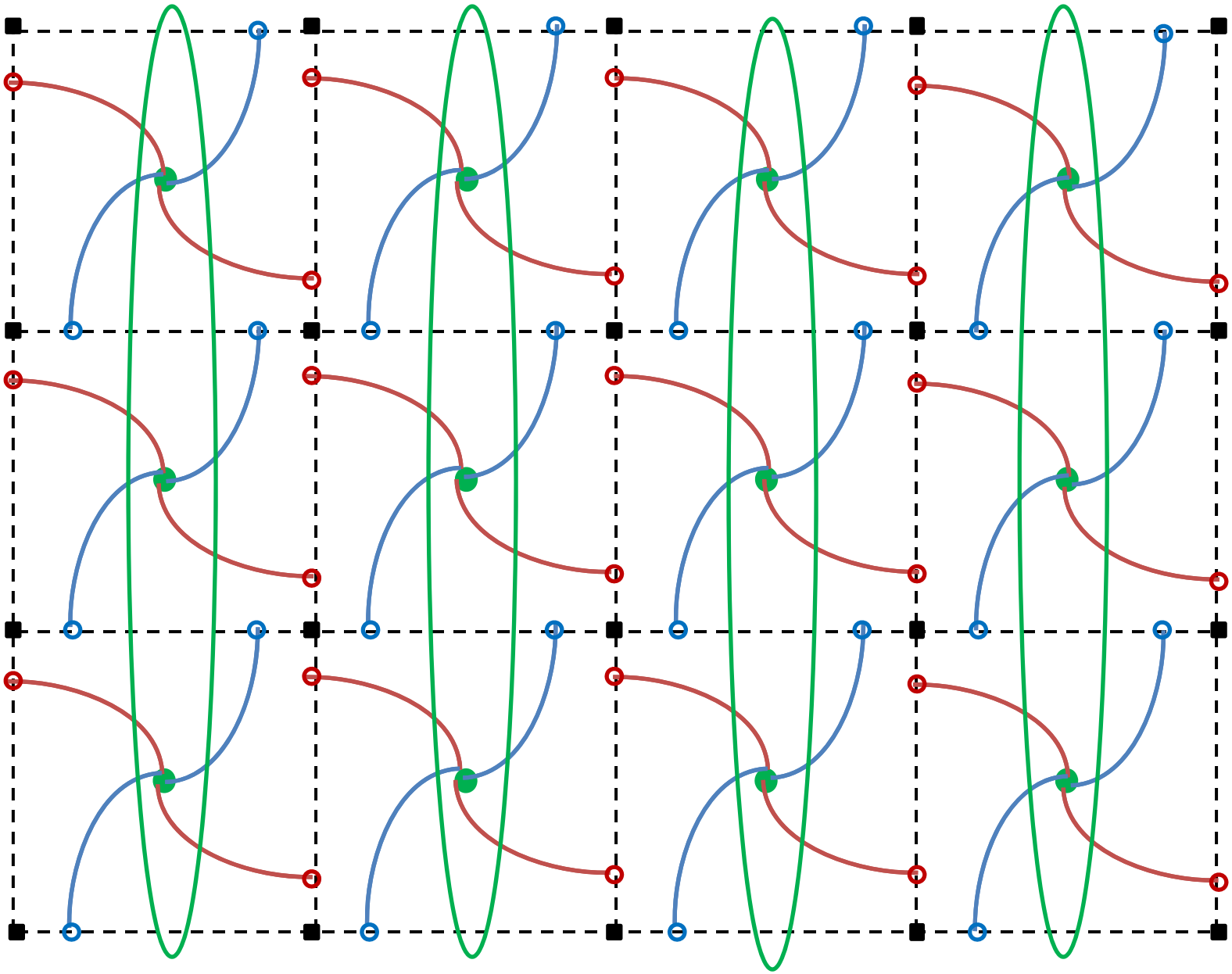
to get f along vertical cell edges.



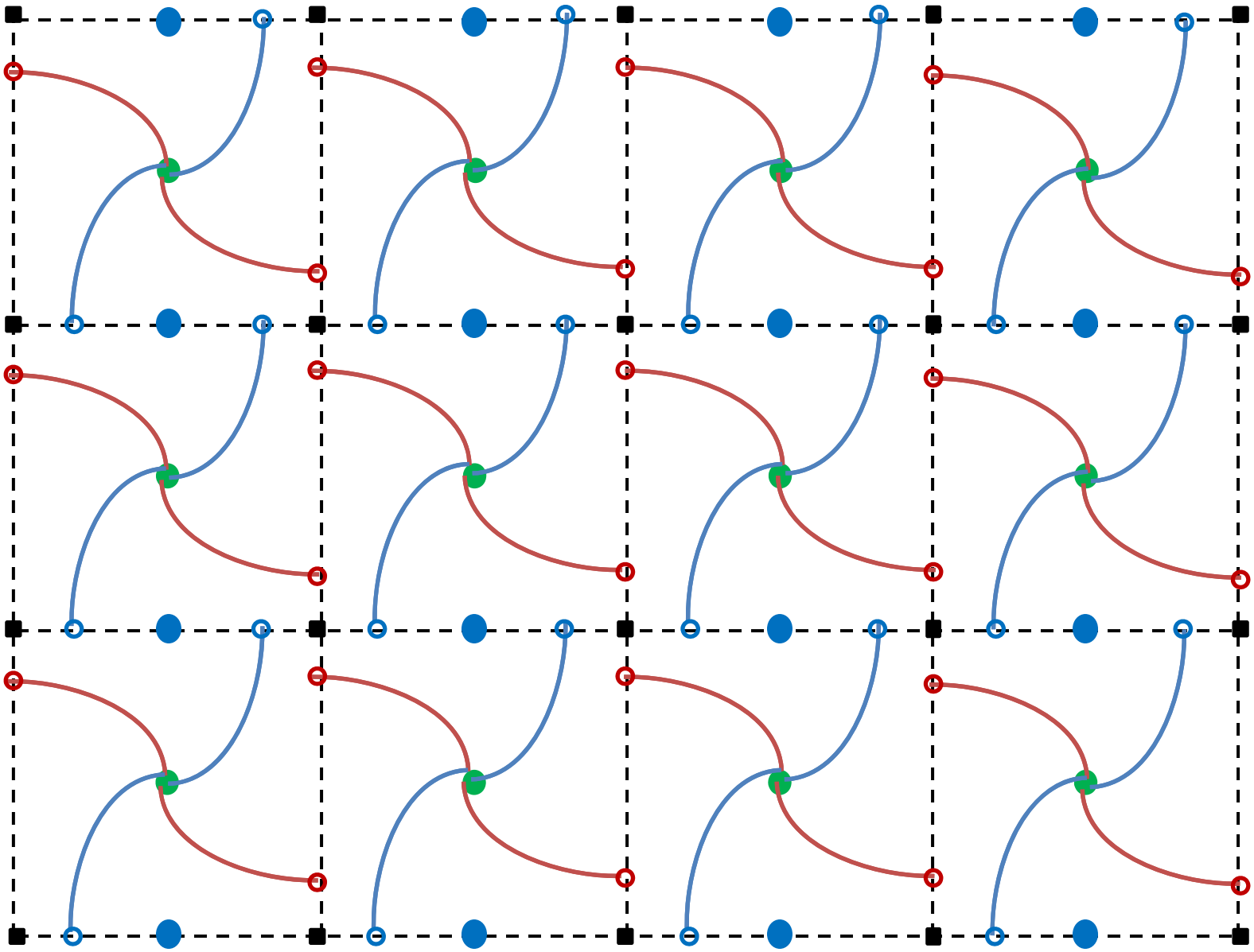
Step 1b: Interpolate f along vertical edges.



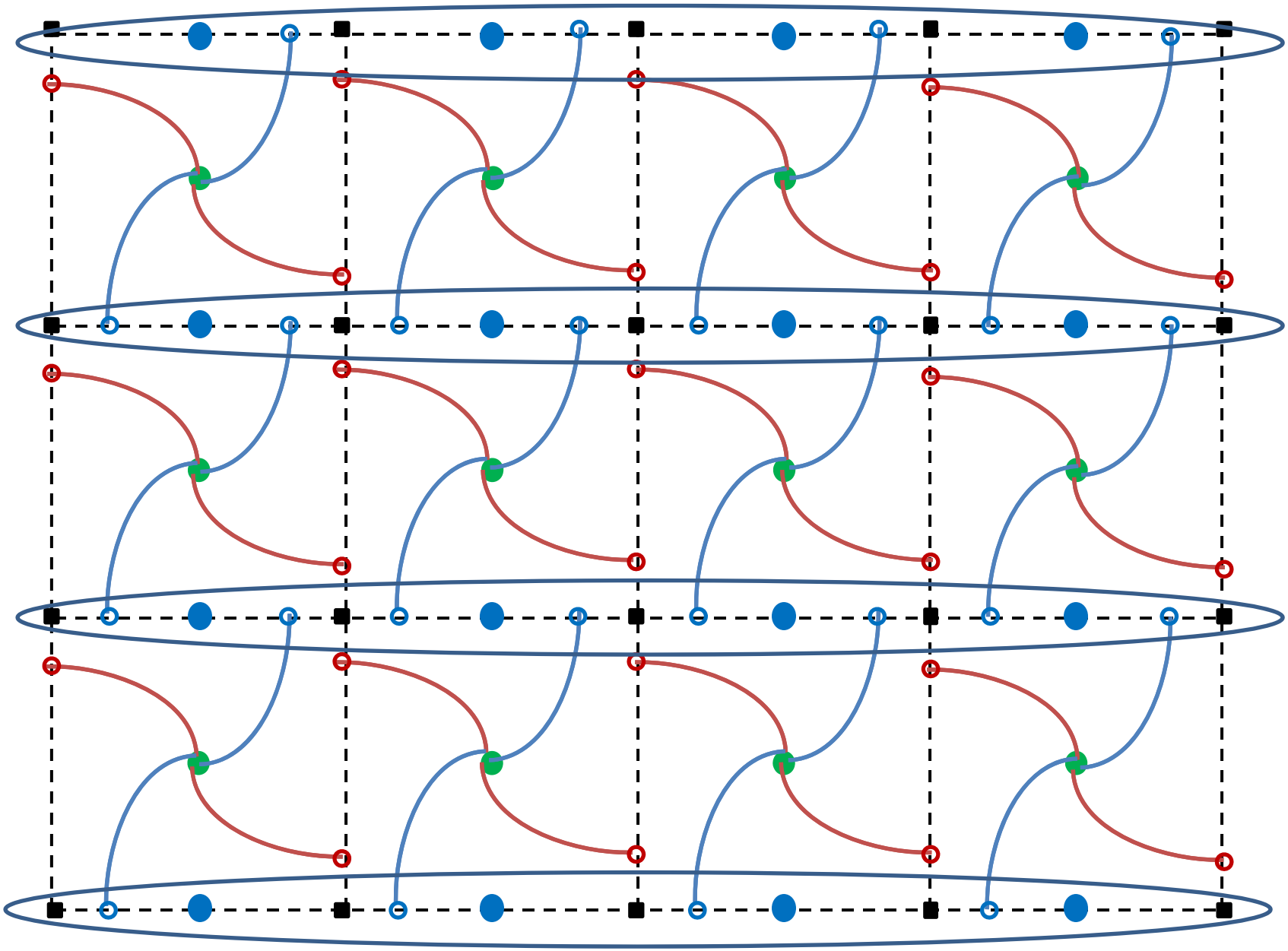
Step 2a: Interpolate f this way …



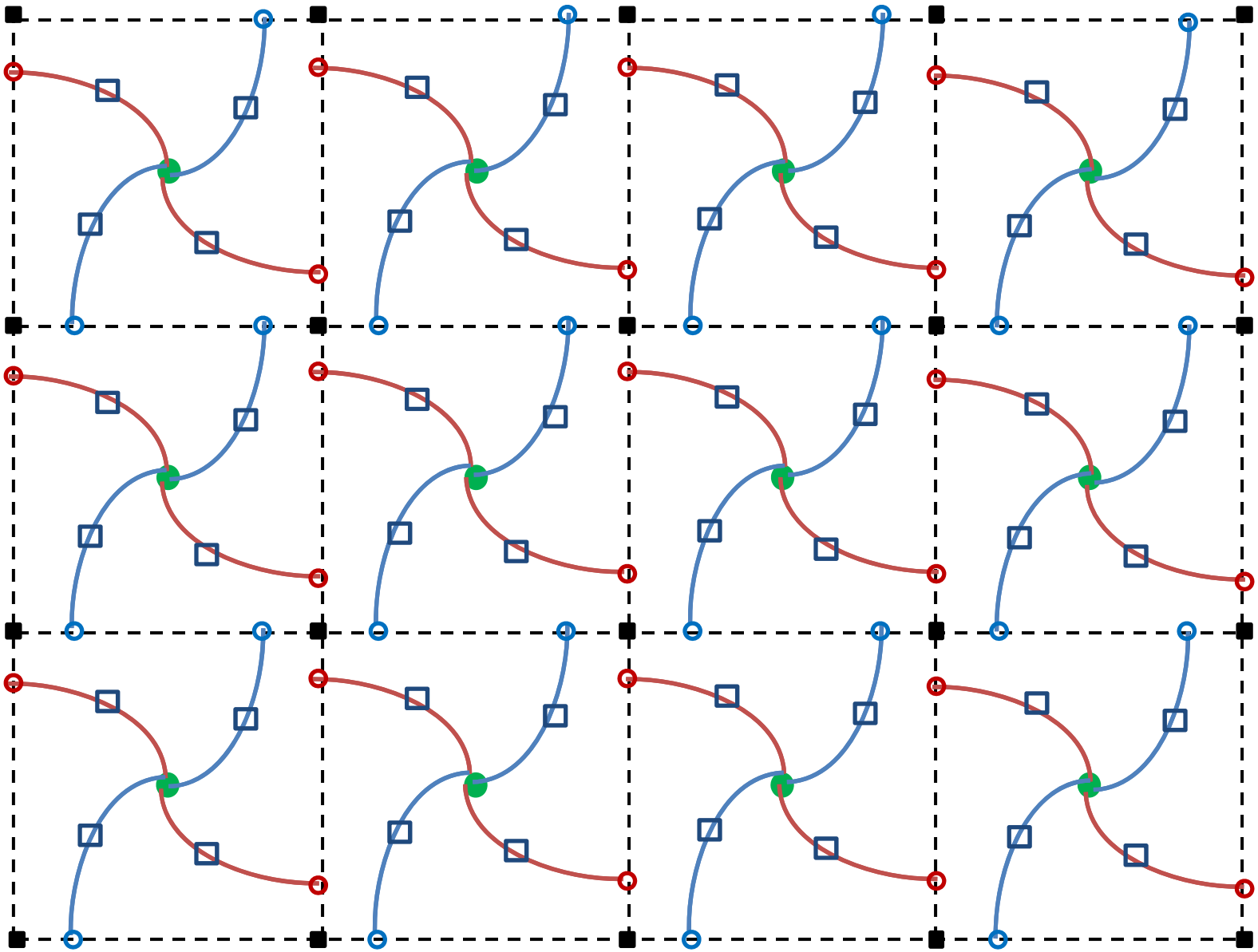
to get f along horizontal cell edges.



Step 2b: Interpolate f along horizontal edges.



Finally, use the interpolated f values in FD scheme. Repeat.



Summary

As with the earlier approach, stability and positivity (f>0) are easily guaranteed.

Using EVs requires tracing both sets of coordinate curves, but give an orthogonal grid. Generalizable to 3D.

Bilinear approximation of D gives closed-form expressions for (Q_1,Q_2) (but requires bilinear approximation of D). Also, coordinate curves don't connect across cells.

PCHIP interpolation in 2D takes a bit of time and trouble, but is better behaved than other methods. Not clear how to combine with implicit time steps.