A free energy satisfying discontinuous Galerkin method for one-dimensional Poisson–Nernst–Planck systems

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1. Introduction

The Poisson–Nernst–Planck (PNP) system, $i = 1, \cdots, m$,

$$\partial_t c_i = \nabla \cdot (\nabla c_i + q_i c_i \nabla \psi) \quad x \in \Omega,\ t > 0 \tag{1a}$$

$$-\Delta \psi = \sum_{i=1}^{m} q_i c_i + \rho_0(x), \quad x \in \Omega,\ t > 0, \tag{1b}$$

$$c_i(0, x) = c_i^{\text{in}}(x), \quad x \in \Omega, \tag{1c}$$

$$\frac{\partial \psi}{\partial \mathbf{n}} = \sigma, \quad \frac{\partial c_i}{\partial \mathbf{n}} + q_i c_i \frac{\partial \psi}{\partial \mathbf{n}} = 0, \qquad x \in \partial\Omega,\ t > 0, \tag{1d}$$

- The Nernst-Planck equation (drift and diffusion)
- The Poisson equation (charge and potential)
- Extensively used in the modeling of semiconductors*, the membrane transport in biological ion channels†, etc.

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* e.g., P. Makowich., C. Ringhofer. and C. Schmeiser. *Springer*, New York, 1990.

† e.g., R. Eisenberg. *Contemp. Phys.*, 39, 1998.

1. Introduction cont'd

- Theoretical results
  - The existence and stability of the steady-state solution, Jerome(1985), etc.
  - Hard to solve analytically due to the nonlinear coupling
- Numerical development (main advance)
  - Many algorithms, including finite difference and finite element methods, are designed in various applications/settings specifically to overcome difficulties such as discontinuous coefficients, singular charges, geometric singularities, etc[‡].
  - In spite of many existing computational studies, rigorous numerical analysis seems to be still lacking.

[‡] e.g., a review by G. Wei., Q. Zheng., Z. Chen. and K. Xia. *SIAM Rev.*, 54(2012).

1. Introduction cont'd

Main mathematical features of the system:

1. conservation of ions,

$$\int_\Omega c_i(t,x)\,dx = \int_\Omega c_i^{\text{in}}(x)\,dx \quad \forall t > 0,$$

2. positivity of concentration,

$$c_i^{\text{in}} > 0 \Longrightarrow c_i > 0 \quad \forall t > 0,$$

3. dissipation of the free energy

$$\frac{d}{dt}F = -\sum_{i=1}^{m}\int_\Omega c_i^{-1}|\nabla c_i + c_i\nabla\psi|^2 dx \leq 0$$

(adjusted by some boundary conditions), where

$$F = \int_\Omega \sum_{i=1}^{m} c_i \log c_i dx + \frac{1}{2}\int_\Omega |\nabla_x \psi|^2 dx.$$

1. Introduction cont'd

Motivation:

- Nonlinear Fokker-Planck (NFP) equations

$$\partial_t c = \nabla_x \cdot (f(c)\nabla_x(\psi(x) + H'(c))). \tag{2}$$

- With external ψ, a direct discontinuous Galerkin (DDG) method introduced[§] satisfies dissipation of free energy discretely.
- If the potential ψ is governed by the Poisson equation, $f(c) = c$ and $H(c) = c \log c$, then NFP becomes the PNP system with single species.

Main objective:

- Develop and analyze a high order DDG method.
- Maintain mathematical features discretely.
- Solution remains faithful for long time simulations,

[§] H. Liu and ZW, J. Sci. Comput., 62 (2015), no. 3, 803–830

2.1 Numerical Scheme: reformulation

We reformulate the PNP system as follows

$$\partial_t c_i = \partial_x (c_i \partial_x p_i), \ i = 1, \cdots, m, \tag{3a}$$

$$p_i = q_i \psi + \log c_i, \tag{3b}$$

$$-\partial_x^2 \psi = \sum_{i=1}^{m} q_i c_i + \rho_0(x), \tag{3c}$$

subject to initial data $c_i(0, x) = c_i^{\text{in}}(x)$ satisfying compatibility condition

$$\int_\Omega \left(\sum_{i=1}^{m} q_i c_i^{\text{in}}(x) + \rho_0(x) \right) dx = \int_{\partial\Omega} \sigma \, ds.$$

2.1 Numerical Scheme: the DDG method

With $V_h = \{v \in L^2(\Omega), \quad v|_{I_j} \in P^k(I_j), j = 1, \cdots, N\}$, the DDG scheme is to find $c_{ih}, p_{ih}, \psi_h \in V_h$, $\forall\ v_i, r_i, \eta \in V_h$, $i = 1, \cdots, m$,

$$\int_{I_j} \partial_t c_{ih} v_i dx = -\int_{I_j} c_{ih} \partial_x p_{ih} \partial_x v_i dx + \{c_{ih}\} \left(\widehat{\partial_x p_{ih}} v_i + (p_{ih} - \{p_{ih}\}) \partial_x v_i \right) \Big|_{\partial I_j},$$

$$\int_{I_j} p_{ih} r_i dx = \int_{I_j} (q_i \psi_h + \log c_{ih}) r_i dx,$$

$$\int_{I_j} \partial_x \psi_h \partial_x \eta dx - \left(\widehat{\partial_x \psi_h} \eta + (\psi_h - \{\psi_h\}) \partial_x \eta \right) \Big|_{\partial I_j} = \int_{I_j} \left(\sum_{i=1}^{m} q_i c_{ih} + \rho_0 \right) \eta dx,$$

with flux $\widehat{\partial_x p_{ih}} = Fl(p_{ih})$ and $\widehat{\partial_x \psi_h} = Fl(\psi_h)$, and

$$Fl(w) := \beta_0 \frac{[w]}{h} + \{\partial_x w\} + \beta_1 h [\partial_x^2 w],$$
$$[w] := w^+ - w^-, \quad \{w\} := (w^+ + w^-)/2$$

Ref: Liu and Yan (SINUM2009, CICP2010).

2.2 Properties: semi-discrete

Theorem

1. *The semi-discrete scheme is conservative in the sense that*

$$\frac{d}{dt}\sum_{j=1}^{N}\int_{I_j} c_{ih}(t,x)dx = 0, \quad t > 0.$$

2. *Suppose* $\partial_t \sigma = 0$ *and* $c_{ih}(t,x) > 0$, *the semi-discrete free energy*

$$F = \sum_{j=1}^{N}\int_{I_j}\left[\sum_{i=1}^{m} c_{ih}\log c_{ih} + \frac{1}{2}\left(\sum_{i=1}^{m} q_i c_{ih} + \rho_0\right)\psi_h\right]dx + \frac{1}{2}\int_{\partial\Omega}\sigma\psi_h ds.$$

$$\frac{d}{dt}F = -\sum_{j=1}^{N}\int_{I_j}\sum_{i=1}^{m} c_{ih}|p_{ihx}|^2 dx - \sum_{j=1}^{N-1}\sum_{i=1}^{m}(\{c_{ih}\}[p_{ih}](\widehat{p_{ihx}} + \{p_{ihx}\}))_{j+1/2}{}^{\P}.$$

Moreover, $\frac{d}{dt}F \le 0$, *provided* β_0 *is suitably large, and* $\beta_1 = 0$ *in* $Fl(\psi_h)$.

$^{\P}:= A_{c_{ih}}(p_{ih}, p_{ih})$, a weighted positive bilinear operator.

2.2 Fully discrete scheme

Using Forward Euler method in time, we have

$$\int_{I_j} D_t c_{ih}^n v_i dx = -\int_{I_j} c_{ih}^n \partial_x p_{ih}^n \partial_x v_i dx + \{c_{ih}^n\} \left(\widehat{\partial_x p_{ih}^n} v_i + (p_{ih}^n - \{p_{ih}^n\}) \partial_x v_i \right) \Big|_{\partial I_j},$$

$$\int_{I_j} p_{ih}^n r_i dx = \int_{I_j} (q_i \psi_h^n + \log c_{ih}^n) r_i dx,$$

$$\int_{I_j} \partial_x \psi_h^n \partial_x \eta dx - \left(\widehat{\partial_x \psi_h^n} \eta + (\psi_h^n - \{\psi_h^n\}) \partial_x \eta \right) \Big|_{\partial I_j} = \int_{I_j} \left[\sum_{i=1}^m q_i c_{ih}^n + \rho_0 \right] \eta dx,$$

with

$$D_t w^n = \frac{w^{n+1} - w^n}{\Delta t}.$$

2.2 Properties: fully discrete

Theorem

1. *The fully discrete scheme is conservative*

$$\sum_{j=1}^{N}\int_{I_j} c_{ih}^{n}dx = \sum_{j=1}^{N}\int_{I_j} c_{ih}^{n+1}dx, \quad i=1,\cdots,m, \qquad t>0.$$

2. *Assuming* $c_{ih}^{n}(x)>0$, *there exists* $\mu^*>0$ *such that if the mesh ratio* $\mu=\frac{\Delta t}{\Delta x^2}\in(0,\mu^*)$, *then the fully discrete free energy*

$$F^n=\sum_{j=1}^{N}\int_{I_j}\left[\sum_{i=1}^{m} c_{ih}^{n}\log c_{ih}^{n}+\frac{1}{2}\left(\sum_{i=1}^{m} q_i c_{ih}^{n}+\rho_0\right)\psi_h^{n}\right]dx+\frac{1}{2}\int_{\partial\Omega}\sigma\psi_h^{n}ds$$

$$D_t F^n \le -\frac{1}{2}\sum_{i=1}^{m} A_{c_{ih}^{n}}(p_{ih}^{n},p_{ih}^{n})$$

Moreover, $F^{n+1}\le F^n$, *provided that* β_0 *is suitably large, and* $\beta_1=0$ *in* $Fl(\psi_h)$.

2.2 Properties: fully discrete cont'd

- The free energy dissipation law is also established for any strong stability preserving Runge-Kutta methods in time
- Preservation of steady states:
  - with initial data c_{ih}^0, already at steady states, i.e., $\log c_{ih}^0 + q_i \psi_h^0(x) = C_i$. By conduction, it is shown that the following holds:
$$\log c_{ih}^n + q_i \psi_h^n(x) = C_i.$$
  - Furthermore, numerical solutions $(c_{ih}^n, p_{ih}^n, \psi_h^n)$ are shown to have the limit
$$p_{ih}^* = C_i, \quad \log c_{ih}^n + q_i \psi_h^n(x) \in C_i + V_h^{\perp},$$
as $n \to \infty$.

2.3 Implementations: Computing unique ψ

- Due to the Neumann Boundary condition, ψ is unique up to an additive constant.
- In order to compute a particular ψ_h, we fix $\psi(a)$ as being given, and define

$$
\begin{aligned}
Fl(\psi_h)(a) &= \beta_0 \frac{(\psi_h^+ - \psi(a))}{h} + \frac{1}{2}(\sigma_a + \psi_{hx}^+), \\
\{\psi\} &= (\psi_h^+ + \psi(a))/2, \\
Fl(\psi_h)(b) &= \sigma_b, \quad \{\psi\} = \psi_h^- .
\end{aligned}
$$

2.3 Implementations: Reconstruction of c_{ih}

- Our algorithm requires c_{ih} being positive point-wise, which is hard to achieve for high order approximation
- For approximation $w_h \in P^k(I_j)$ with cell averages $\bar{w}_j > \delta$, we reconstruct

$$w_h^\delta(x) = \bar{w}_j + \frac{\bar{w}_j - \delta}{\bar{w}_j - \min_{I_j} w_h(x)}(w_h(x) - \bar{w}_j), \qquad \text{if } \min_{I_j} w_h(x) < \delta.$$

This reconstruction

  - maintains same cell averages,
  - satisfies $\min_{I_j} w^\delta(x) \geq \delta$,
  - does not destroy accuracy when $\delta < h^{k+1}$

2.3 Implementations: Algorithm

The algorithm can be summarized in following steps.

1. (Initialization) Project $c_i^{\text{in}}(x)$ onto V_h to obtain $c_{ih}^0(x)$.
2. (Reconstruction) From $c_{ih}^n(x)$, apply, if necessary, the reconstruction to c_{ih}^n to ensure that in each cell $c_{ih}^n > \delta$.
3. (Poisson solver) Solve Poisson equation to obtain ψ_h^n subject to the modified boundary fluxes
4. (Projection) Obtain p_{ih}^n.
5. (Update) Solve NP equation to update c_{ih}^{n+1} with some Runge-Kutta ODE solver.
6. Repeat steps 2-5 until final time T.

3. Example 1: Cell average and convergence test

$$
\begin{aligned}
\partial_t c_1 &= \partial_x(\partial_x c_1 + q_1 c_1 \partial_x \psi) + f_1, \\
\partial_t c_2 &= \partial_x(\partial_x c_2 + q_2 c_2 \partial_x \psi) + f_2, \\
-\partial_x^2 \psi &= q_1 c_1 + q_2 c_2, \\
\partial_x \psi(t,0) = 0, &\quad \partial_x \psi(t,1) = -e^{-t}/60, \\
\partial_x c_i + q_i c_i \partial_x \psi &= 0, \quad x = 0, 1,
\end{aligned}
$$

$$
\begin{aligned}
f_1 &= (50x^9 - 198x^8 + 292x^7 - 189x^6 + 45x^5)e^{-2t}/30 \\
&\quad + (-x^4 + 2x^3 - 13x^2 + 12x - 2)e^{-t}, \\
f_2 &= (x-1)(110x^9 - 430x^8 + 623x^7 - 393x^6 + 90x^5)e^{-2t}/60 \\
&\quad + (x-1)(x^4 - 2x^3 + 21x^2 - 16x + 2)e^{-t}.
\end{aligned}
$$

This system, with $q_1 = 1$ and $q_2 = -1$, admits exact solutions

$$
\begin{aligned}
c_1 &= x^2(1-x)^2 e^{-t}, \quad c_2 = x^2(1-x)^3 e^{-t}, \\
\psi &= -(10x^7 - 28x^6 + 21x^5)e^{-t}/420.
\end{aligned}
$$

3. Example 1: Cell average and convergence test cont'd

Table: Error table at $T = 0.1$

(k, β_0, β_1)	h	c_1 error	order	c_2 error	order	ψ error	order
$(1, 2, -)$	0.2	0.0232	–	0.0312	–	0.0033	–
	0.1	0.0037	2.50	0.0059	2.26	0.0009	1.86
	0.05	0.0006	2.44	0.0012	2.19	0.0002	1.87
	0.025	0.0001	2.36	0.0002	2.13	6.98e-5	1.90
$(2, 4, 1/12)$	0.2	0.0028	–	0.0030	–	0.0012	–
	0.1	0.0001	3.64	0.0002	3.44	0.0001	3.46
	0.05	1.39e-5	3.49	2.27e-5	3.34	9.14e-6	3.38
	0.025	1.48e-6	3.23	2.42e-6	3.23	9.24e-7	3.31
$(3, 15, 1/4)$	0.2	0.0030	–	0.0029	–	0.0011	–
	0.1	0.0002	4.07	0.0002	3.93	7.41e-5	4.39
	0.05	1.75e-5	4.24	1.68e-5	4.01	5.41e-6	4.64
	0.025	6.44e-7	4.76	8.33e-7	4.33	1.19e-7	5.50

All cell average are positive at $T = 100$

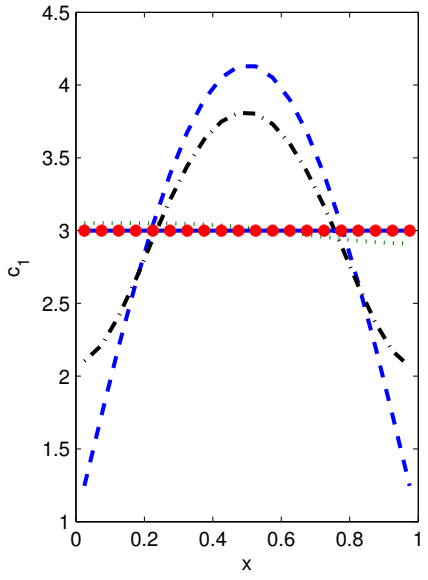
3. Example 2: Mass and free energy

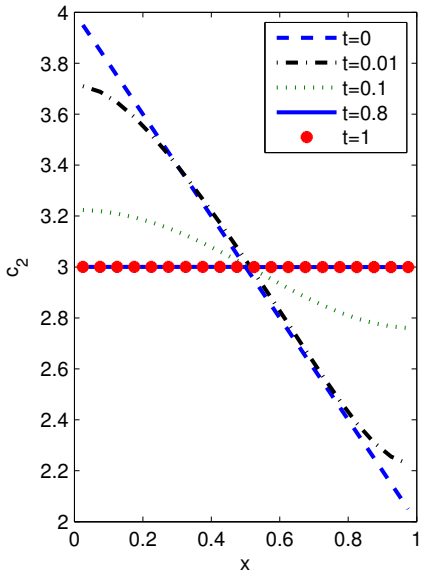
$$\begin{aligned} \partial_t c_i &= \partial_x(\partial_x c_i + q_i c_i \partial_x \psi), \quad i = 1, 2 \\ -\partial_x^2 \psi &= q_1 c_1 + q_2 c_2, \\ \partial_x \psi = 0, \quad \partial_x c_i &= 0, \quad i = 1, 2, \quad x = 0, 1, \end{aligned}$$

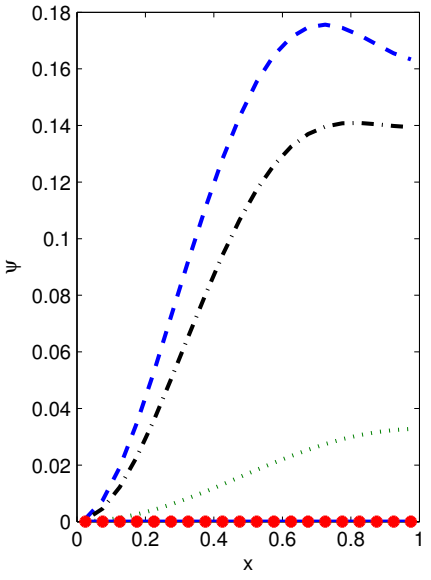
where q_1 and q_2 are set to be 1 and -1, respectively, with initial conditions

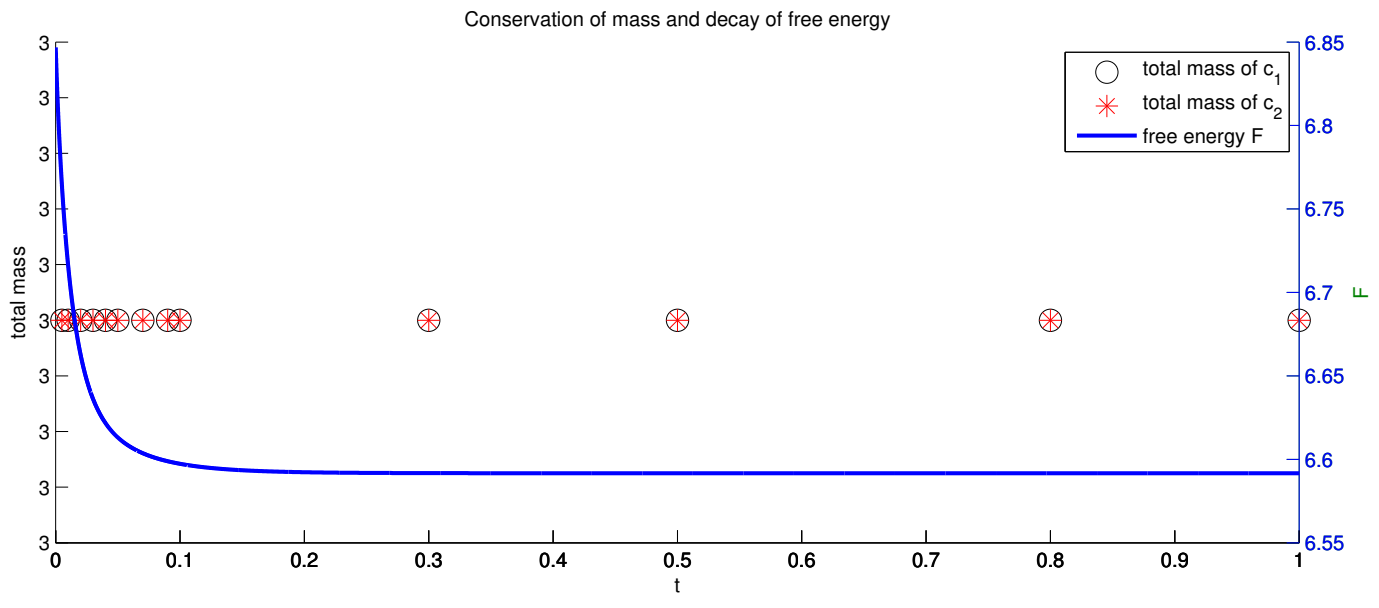
$$c_1^{\text{in}}(x) = 1 + \pi \sin(\pi x), \quad c_2^{\text{in}}(x) = 4 - 2x,$$

3. Example 2: Mass and free energy dissipation cont'd









3. Example 3: Non-monovalent and nonzero ρ_0

$$\begin{aligned}
\partial_t c_1 &= \partial_x(\partial_x c_1 + q_1 c_1 \psi_x),\\
\partial_t c_2 &= \partial_x(\partial_x c_2 + q_2 c_2 \psi_x),\\
-\partial_x^2 \psi &= q_1 c_1 + q_2 c_2 + \rho_0,
\end{aligned}$$

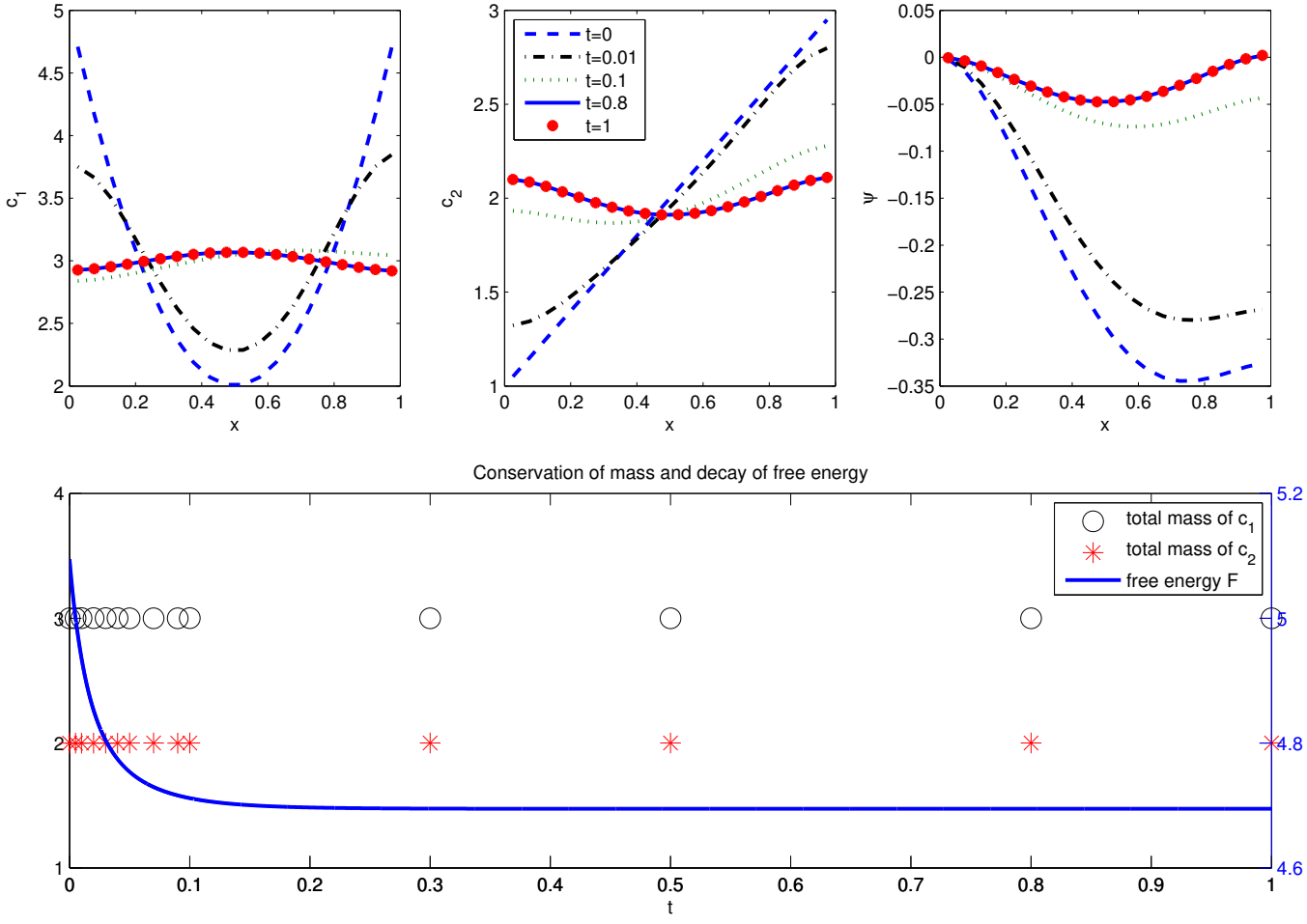
with $q_1 = 1$, $q_2 = -2$ and $\rho_0 = 12(x - 0.5)^2$. The initial and boundary conditions are

$$\begin{aligned}
c_1^{\text{in}}(x) = 2 + 12(x - 0.5)^2, \quad c_2^{\text{in}}(x) = 1 + 2x,\\
\partial_x c_i + q_i c_i \partial_x \psi = 0, \quad x = 0, 1,\\
\partial_x \psi(t, 0) = \partial_x \psi(t, 1) = 0,
\end{aligned}$$

where the compatibility condition (**??**) is satisfied since

$$\int_0^1 (q_1 c_1^{\text{in}} + q_2 c_2^{\text{in}} + \rho_0) dx = 0.$$

3. Example 3: Non-monovalent and nonzero ρ_0 cont'd



4. Summary and Future Work

Summary

- An arbitrary high order DDG method for the PNP system
- Both semi-discrete and fully DDG schemes (later with the Euler forward time discretization) are shown to satisfy mass conservation and discrete free energy dissipation
- The method also preserves the steady states.
- For proper choices of (β_0, β_1), we numerically confirm that each cell average remains positive in long time.

Future work

- Multi-dimensional extension
- New ideas on preserving positivity of numerical cell average

Thank you!