Classical Transport Models Beyond PNP: Results and Questions

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Transport of Ionic Particles in Biological Environments
Fields Institute
July 30, 2014

Introduction

This talk discusses classical models more comprehensive than standard PNP models for ion transport.

- For the first part of the talk, we will review:
  1. One-Fluid/Ionic transport model (Rubinstein model);
  2. Hydrodynamic model (three-moment model: BBW).
- For the second part, we summarize results for a gating model, and, separately, for some energy transport models.
- For the third part, we wish to consider briefly the challenging model related to ‘crowded ions’, and discuss why standard analysis does not appear to be successful for this model.

For parts one and two, we raise some questions: relevance of the models and resolution of analytical issues. These models do not include finite size particle potentials.

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Rubinstein Model for Nonlinear Electrophoresis

The ions are considered as points, and the fluid has no nematic phases. The constitutive relations for the current densities extend the usual relations by the inclusion of *velocity convection* terms [I. Rubinstein, SIAM, 1990].

- $\mathbf{v}$ is the velocity of the electrolyte, and the anion and cation concentrations are n, p, respectively.
- The current densities are (Generalized Ohm's Law):

$$\mathbf{J}_n = eD_n\nabla n - e\mu_n n\nabla\phi \boxed{-e\mathbf{v}n}, \quad (1)$$

$$\mathbf{J}_p = -eD_p\nabla p - e\mu_p p\nabla\phi \boxed{+e\mathbf{v}p}. \quad (2)$$

  Here, J_n, J_p are the anion and cation current densities, with corresponding (constant) diffusion and mobility coefficients, D_n, D_p, μ_n, μ_p, respectively. Displacement current is neglected.
- The charge modulus is e.
- ϕ is the electric potential.
- The Poisson equation describes the coupling.

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Enhanced PNP Subsystem

The enhanced PNP system is, with ϵ the dielectric:

$$\frac{\partial n}{\partial t} - \frac{1}{e}\nabla\cdot\mathbf{J}_n = 0, \tag{3}$$

$$\frac{\partial p}{\partial t} + \frac{1}{e}\nabla\cdot\mathbf{J}_p = 0, \tag{4}$$

$$\mathbf{E} = -\nabla\phi, \tag{5}$$

$$\nabla\cdot(\epsilon\nabla\phi) = e(n-p) + \boxed{\rho_0} \quad \text{(Poisson equation)}. \tag{6}$$

- The Einstein relations are employed: $D_n = (kT_0/e)\mu_n, D_p = (kT_0/e)\mu_p$.
- Here, T_0 is the ambient temperature; k denotes Boltzmann's constant. ρ_0 is the fixed charge, when present.
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Navier-Stokes Subsystem

The velocity of the electrolyte is determined by the Navier-Stokes equations (with volume force included):

$$m(\mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v}) - \eta\nabla^2\mathbf{v} = -\nabla P_f \boxed{-e(p-n)\nabla\phi}, \tag{7}$$

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- Dirichlet velocity boundary condition is specified, which extends the no-slip condition: it must be outward pointing.
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Status of Results

- Computationally feasible for both the dynamic and steady cases. There is an iteration map which switches:
  1. The PNP part uses a Gummel type solution, and updates concentrations and electric field.
  2. The Navier-Stokes subsystem uses fixed point iteration based on Oseen sub-problem solutions; the velocity and pressure are updated. [(CJLS) J. Comp. Elect. 7, 10-13 (2008)].

Theorem

(1) For the dynamic model, there is a local smooth solution theory for the Cauchy problem, and a global weak solution theory for the initial mixed boundary value problem. Concentrations are non-negative.
(2) There exists a weak solution to the steady problem under (relative) assumptions on domain size. A maximum principle is derived for the concentrations.

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Highlights I

Model relevance:

1. The significance of fluid motion on current density is still an open question in the range of physiological parameters.
2. It is known that a specified pressure drop of approximately one atmosphere across a (VOC–K^+) channel leads to enhanced current densities at the ends of the channel.
3. The Rubinstein model may be more relevant when connected (as in a bio-chip) to a transistor sensing device (Fromhertz model), or in the study of electro-osmosis.

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Highlights II

Mathematical model:

1. A local smooth solution result for the Cauchy problem was obtained via (equivalent of) evolution operators. [J, Trans. Th. Stat. Phys. 31, 333-366 (2002)]. The interval of existence/uniqueness was shown stable under vanishing viscosity $\eta \longrightarrow 0$.
2. There are several results for the initial/boundary-value problem.
   - Rubinstein model: [JS, Nonlinear Anal. 71, e2487-e2497 (2009)]. [M. Schmuck, MMM Appl. Sc. 19, 993-1015 (2009)]. [R. Ryham, ArXiv preprint (2009)].
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General Comments on the Hydrodynamic Model

- In 1970, Bløtekjaer introduced a moment model for semiconductors with two energy valleys, using the Boltzmann equation as the basic kinetic equation (hydrodynamic scaling).
- The model is consistent with extended thermodynamics, in the sense that that the Maxwell-Boltzmann distribution is a stationary distribution for the entropy functional, subject to the three derived moment constraints.
- Later choices of the heat flux, and the approximation of collision terms are seen as ‘ad hoc’, however.
- The moment model, together with the choice of these approximations is called the Bløtekjaer-Baccarani-Wordeman model (BBW).
- There is a very clear discussion of the model in the thesis of Cory Hauck (2006), written under the direction of C. David Levermore. Several of Levermore’s contributions to higher moment models (1990s) are explained in the thesis.

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Bløtekjaer-Baccarani-Wordeman Model

This model views the charges as a compressible fluid. Its main features are the following (specialized to one carrier).

- It is based upon three moments of a kinetic equation (Boltzmann equation), leading to four equations (including the Poisson equation) for fifteen unknowns.
- The unknowns are moments of a numerical distribution function: n (carrier density); $\mathbf{v}$ (carrier velocity); P (symmetric pressure tensor); $\mathbf{q}$ (heat flux); w (energy density); and, ϕ (electric potential).
- Constitutive relations are chosen for P, $\mathbf{q}$, w in order to close the moment system.
- P is assumed isotropic, of the form $\mathrm{P}_{ij} = P\delta_{ij}$, where P satisfies the ideal gas law.
- $\mathbf{q}$ satisfies the Fourier law, with a concentration-dependent conductivity (Wiedemann-Franz law).
- w is defined by an internal energy component and a parabolic band kinetic energy component.

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Expressions for Heat Flux and Relaxation

- Wiedemann-Franz law: $\kappa = \kappa_0 n$. As derived, κ_0 includes an adjustable parameter, which varies between $5/2$ and 0.
- Heat flux law: $\mathbf{q} = -\nabla(\kappa T)$.
- The momentum and energy equations possess collision moments; they incorporate friction, via relaxation times (τ_p, τ_w). The relaxation approximations of the collision moments are:

$$\begin{aligned} C_p &= -n\mathbf{v}/\tau_p, \\ C_w &= -\frac{w - w_0}{\tau_w}, \\ \tau_p &= c_p/T, \\ \tau_w &= \frac{\tau_p}{2} + c_w \frac{TT_*}{v_s^2(T + T_*)}. \end{aligned}$$

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$$\begin{aligned} C_p &= -n\mathbf{v}/\tau_p, \\ C_w &= -\frac{w - w_0}{\tau_w}, \\ \tau_p &= c_p/T, \\ \tau_w &= \frac{\tau_p}{2} + c_w \frac{TT_*}{v_s^2(T + T_*)}. \end{aligned}$$

- c_p, c_w are physical constants; v_s is the saturation velocity. T_* is the equilibrium temperature.

Expressions for Heat Flux and Relaxation

- Wiedemann-Franz law: $\kappa = \kappa_0 n$. As derived, κ_0 includes an adjustable parameter, which varies between $5/2$ and 0.
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System: Non-conservative Friedrichs Form

For the dependent variables n, $\mathbf{v}$, and T, the non-conservative form of the system is helpful for analysis:

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$$T_t - \frac{\kappa_0}{n}\nabla\cdot(n\nabla T) + \mathbf{v}\cdot\nabla T + \frac{2}{3}T\nabla\cdot\mathbf{v} = -\frac{2m|\mathbf{v}|^2}{3k}\left(\frac{1}{2\tau_w} - \frac{1}{\tau_p}\right) - \frac{T - T_*}{\tau_w}.$$

The system admits of a symmetrizing matrix multiplier, in the sense of Friedrichs, and can be analyzed in this manner. The undefined constants are: k (Boltzmann's constant); m (carrier mass).

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Effect of Saturation Velocity v_s

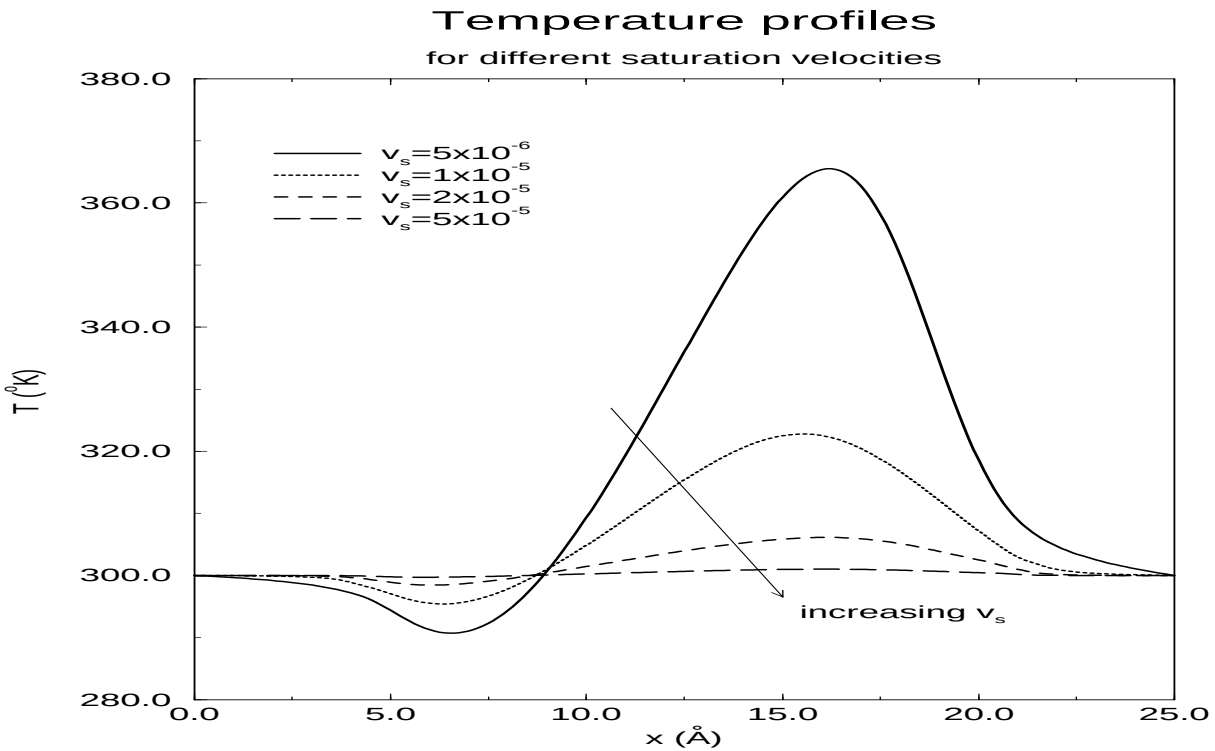

Figure: The solid curve gives the temperature for $v_s = 5 \times 10^{-6}$, the dotted curve is for $v_s = 10^{-5}$, the short-dashed curve is for $v_s = 2 \times 10^{-5}$, and the long-dashed curve is for $v_s = 5 \times 10^{-5}$. The decrease of temperature coincides with efficient damping of energy exchange. τ_W depends inversely on v_s^2. The units of v_s are μm/ps. From [CEJS].

Global Solutions and Relaxation Limit

It is natural to ask the following two questions:

1. Can one strengthen the local existence result cited earlier?
2. Can one establish analytically a drift-diffusion limit as relaxation times tend to zero?

'Yes' to both questions in *one* dimension for electrically neutral boundary conditions for ϕ. [(CJZ) Chap. 9, Modelling and Computation for Applications in Mathematics, Science, and Engineering, Oxford Press (1998)].

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Methodology for Incompletely Parabolic Systems

The results cited for the Cauchy problem (both Rubinstein and BBW models) depend on *non-parabolic* methods. This permits:

- The time interval for smooth solutions of the BBW model remains invariant as $\kappa \to 0$.

Methods for parabolic problems typically experience blow-up when 'de facto' diffusion is eliminated from the system.

- The underlying theory was developed by Kato in the 1970s, and uses semi-groups of operators.
- The key idea is that the semi-groups are generated on a ground space X, but remain invariant on a smooth (relative to X) space Y.
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Phase Space Orbits

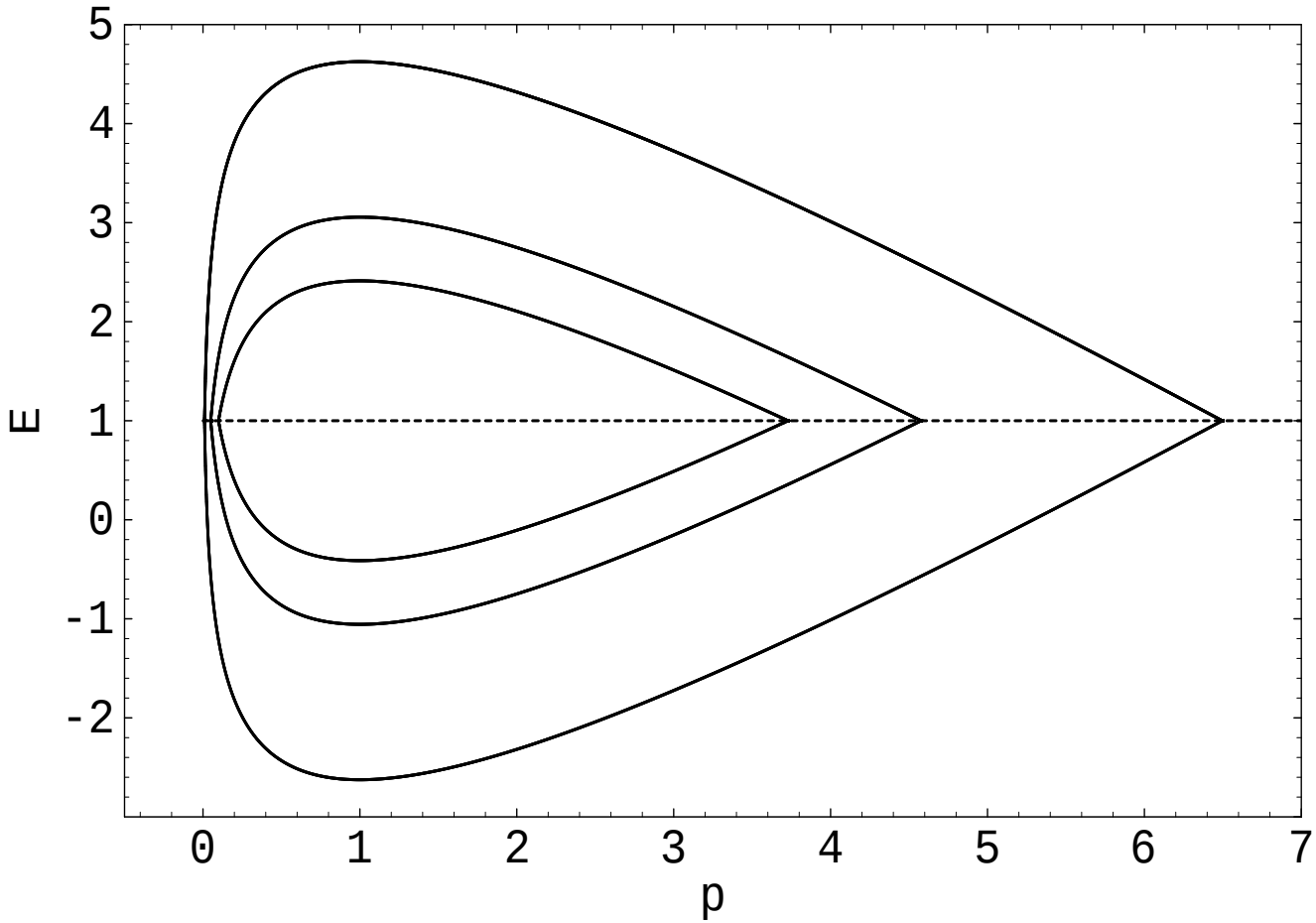

Figure: Heteroclinic orbits in phase space $(p/\overline{p}, E/\overline{E})$ for different initial conditions p_0, E_0. The line of fixed points is also shown. Reproduced from [GJE].

Flat Top Time Profiles

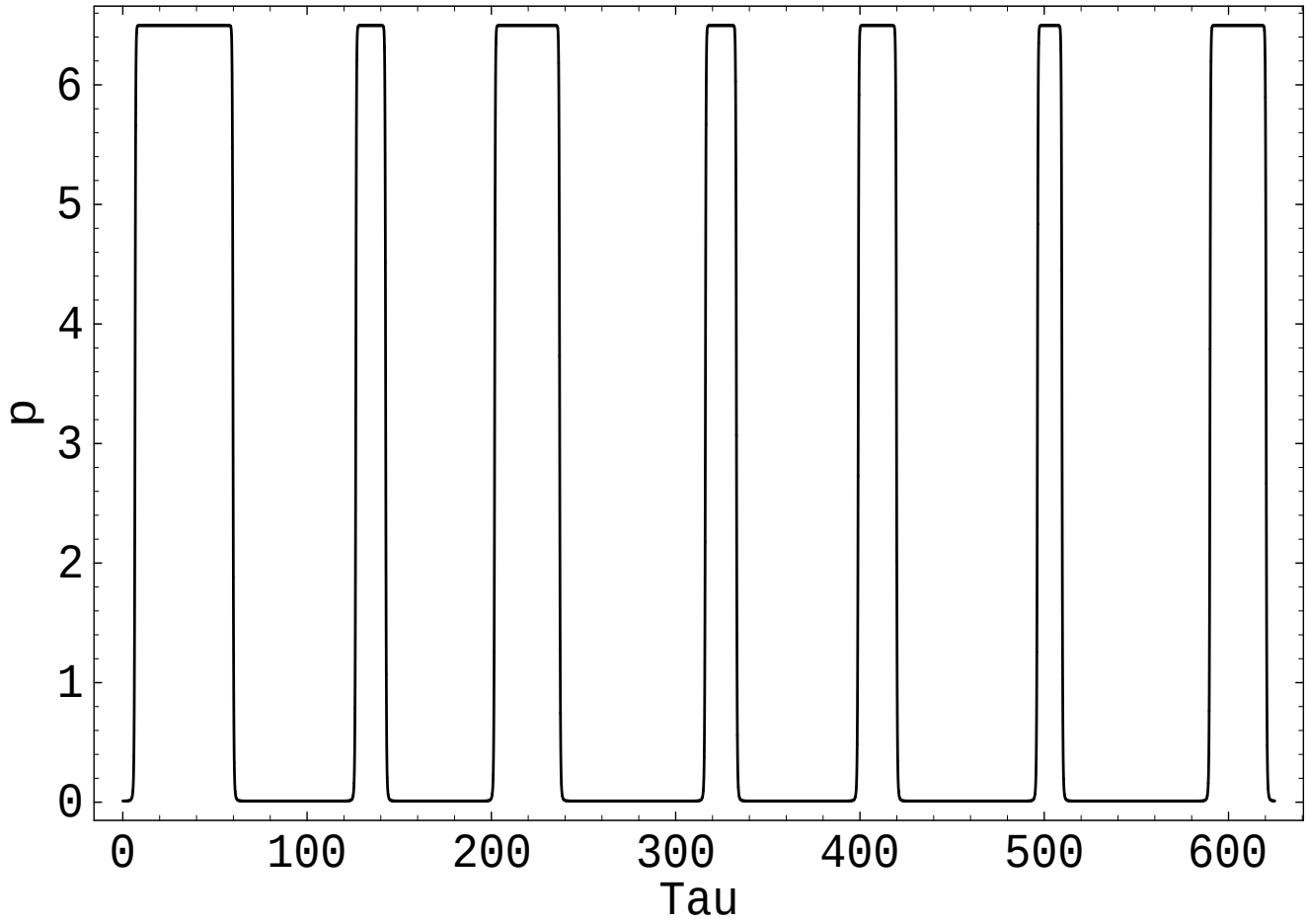

Figure: Solution $p/\overline{p}$ vs. $\tau\overline{E}$ with random noise added every thousandth timestep on average. Reproduced from [GJE]

System for the Deterministic Finite Channel

For a finite channel located on $[a, b]$, transporting a cation carrier:

$$\frac{\partial p}{\partial t} + \frac{1}{e}\frac{\partial j}{\partial x} = 0,$$
$$\frac{\partial}{\partial x}(\varepsilon E) = e(p - \rho_0) = \rho(p, E),$$

The net charge density $e(p - \rho_0)$, combining the mobile ions with the charge on the protein, is expressed by:

$$\rho(p, E) = -ce(p - \bar{p})\left|\frac{E}{\bar{E}} - 1\right|,$$

where $c, \bar{p}, \bar{E}$ are positive constants; $\bar{p}, \bar{E}$ are reference levels. The formula was derived by Gardner, via a Boltzmann factor [pp. 794–795]. Boundary and initial conditions are:

$$p(a, t) = p_a(t),\ p(b, t) = p_b(t),\ E(a, t) = E_a(t),\ \phi(b, t) = \phi_b(t),$$
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Results and Remarks

- The minus sign is critical for gating. Simulations show that rectangular pulses are not observed if $\rho \mapsto -\rho$ for positive ions; there is a type of mirror symmetry for negative charges, and in this case one obtains rectangular pulses for $\rho \mapsto -\rho$ and negative $\bar{E}$.
- The results depend strongly on the derivation of invariant region principles. The following hypothesis is directly tied to this fact:
- *The supremum norms of p_a, p_b, p_0 do not exceed $\bar{p}$.*
- The article [Dis. Cont. Dyn. Sys. 17, 2465-2482 (2012)]. derives existence and uniqueness, and establishes that $\bar{p}$ is a bound for p when the data satisfy this condition. This corresponds to the channel state when the field is increasing.
- It is an open question as to the case when the field is decreasing.
- Is there a connection to binding and unbinding of ions? [(Siwy, Powell, Petrov, Kalman, Trautmann, Eisenberg) Nanoletters 6, 1729-1734 (2006)].

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Crowded Ions Model

By including dissipation proportional to the square of the relative carrier velocity, [(Hsieh, Hyon, Lee, Lin, Liu), (2013)] have derived an extended PNP model and proven a local existence/uniqueness result, including nonnegative properties for the concentrations c_n, c_p. The system reads,

$$\frac{\partial c_n}{\partial t} = \nabla \cdot \left[\frac{1}{1+c_n+c_p} \left((1+c_n)(\nabla c_n - c_n \nabla \phi) + c_n (\nabla c_p + c_p \nabla \phi) \right) \right]$$

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Non-Coerciveness

The key property missing in the spatial part of the operator is coerciveness; this makes the analysis very challenging. The non-coerciveness of the system is induced by the quadratic form,

$$A|\nabla c_n|^2 - (A+B)|\nabla c_n||\nabla c_p| + B|\nabla c_p|^2,$$

where each term is a function of space and time. The functions A and B are derived from the input (boxes). It can be shown that a sharp lower bound is given by,

$$-\frac{1}{4}|A-B|(|\nabla c_n|^2 + |\nabla c_p|^2)$$

which indicates that this expression can be negative. This explains the lack of the coerciveness property.
One does have *Galerkin coerciveness*.

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Conjecture and Comments

A preliminary analysis suggests the following conjecture.

- Rothe's method, combined with a spatial Galerkin method on each time subinterval, leads to a convergent space-time sequence for the linear *output* problem.

1. This is a fully discrete characterization of approximation of the linear problem.
2. This is preliminary to the local fixed point analysis.
3. Are there any biophysical implications of the fact that the result is local?
4. This represents a *new frontier* for PNP modeling!

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