Use of Field Theories in Chemical Process Modeling

Canonical Primal-Dual Form, Practical Reductions, and Problem Specifications

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136b AIChE Atlanta November 17, 2014

Modeling Issues (steady state)

Representation of physical situation

- Phenomenology
- Geometries (structure)
- Modularization

Specifications (parametric)

- Formulation consistency
- Allowable options
- Admissible, v.s. Goals

Detail: abstraction $\longleftrightarrow$ refinement

Unification: steady state – dynamic – optimization

Numerical solution

Incremental Path Forward ?

Sequential modular

"Equation-based/oriented"

25 years ?

Roadblock: 1 Convergence

10 k nonlinear algebraic

(2 Modeling skill)

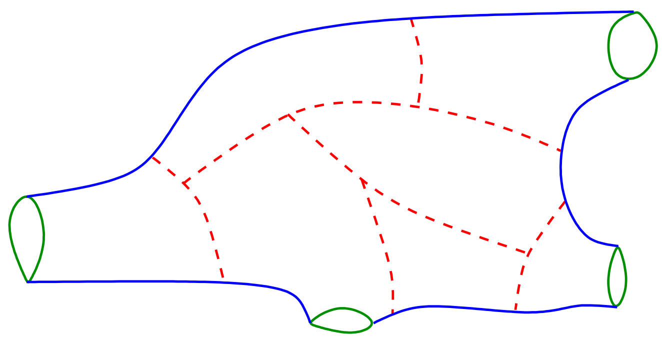
Old paradigm: Physical Situation — "Model" → Algebraic Equations — "Solve" → Numerical Algorithm

~~Improving "numerical methods"~~ → Rethink & Re-do

How Does Nature Do It? ← Field Principles

Physics: Field Theories

Continuum description: Continuous fields in space



Variational principle

$$S = \int d^4x \; \mathcal{L}(\psi, \nabla\psi, x)$$

mechanics

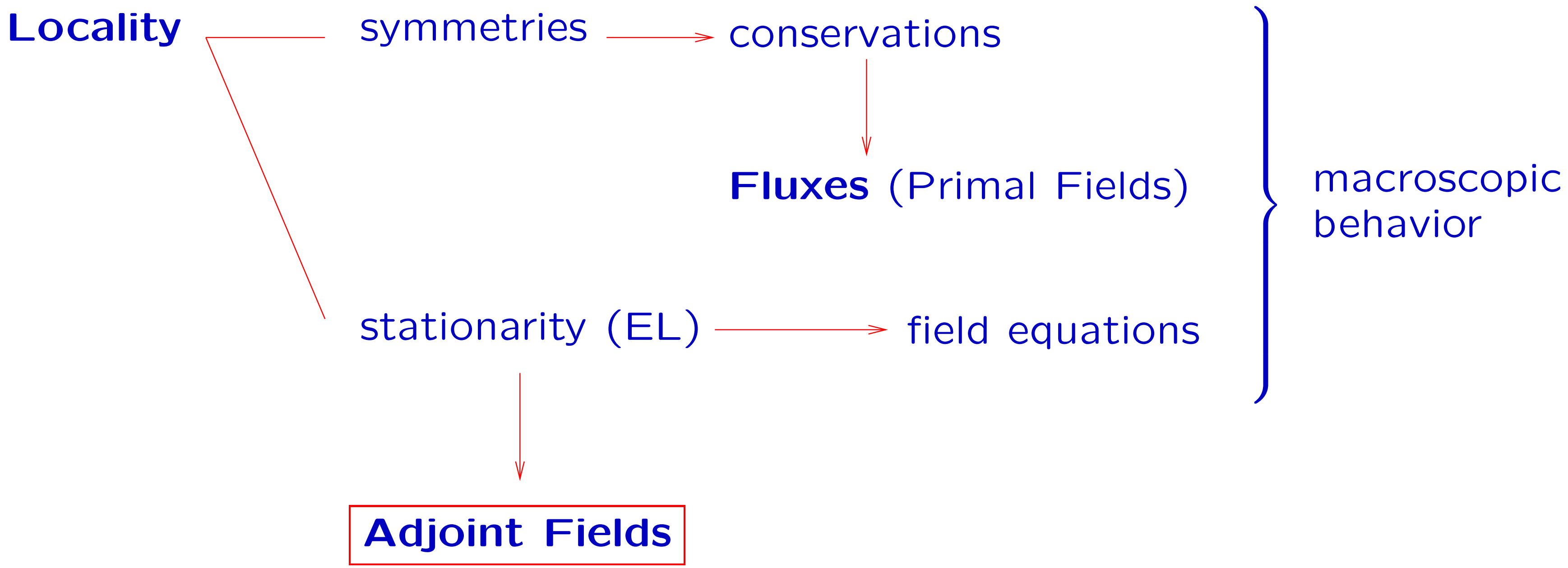
gauge theories

gravitation

$\vdots$

$\min S$

(+ invariance symmetries)


Locality
symmetries
conservations
Fluxes (Primal Fields)
macroscopic
behavior
stationarity (EL)
field equations
Adjoint Fields

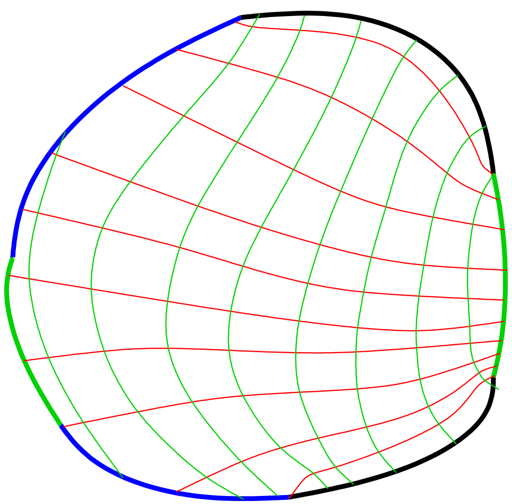
conservations + EL → 2nd order PDEs

↓ 2nd Law (directionality)

Elliptic system

↓

Potential Theory



Uniqueness principle

Divergence theorem

↓

Integrating — surface ↕ volume

Physics at a point

Macroscopic	*Microscopic*
Dissipation + Couplings + Reactions	LE thermodynamics transport kinetics

Fields: Conserved densities (fluxes) & adjoint potentials

Conservation	Flux			Potential
	Transport j^α	Coupling σ^α	Reaction r^k	
Species	$\mathbf{j}^i = \mathbf{J}^i + \rho^i \mathbf{v}$	-	$\sum_k \nu_i^k r^k$	λ^i
Energy	$\mathbf{j}^{\mathsf{E}} = \mathbf{J}^{\mathsf{E}} + \rho^{\mathsf{E}} \mathbf{v}$	σ^{E}	-	λ^{E}
Momentum	$\mathbf{j}^{\mathbf{p}} = \mathbf{J}^{\mathbf{p}} + \rho^{\mathbf{p}} \mathbf{v}$	$\sigma^{\mathbf{p}}$	-	$\lambda^{\mathbf{p}}$
Strain	$\mathbf{j}^{\mathbf{F}} = \mathbf{J}^{\mathbf{F}} + \rho^{\mathbf{F}} \mathbf{v}$	$\sigma^{\mathbf{F}}$	-	$\lambda^{\mathbf{F}}$

Diffusion/convection model

Variational form

$$\min_{j^\alpha,\sigma^\alpha,r^k} \iiint_V \sigma^S dV = \iiint_V \left(\begin{bmatrix} j^\alpha \\ \sigma^\alpha \\ r^k \end{bmatrix}^T R \left[j^\alpha, \sigma^\alpha, r^k \right] \right) dV$$

$$\text{s.t.} \quad \nabla \cdot \mathbf{j}^\alpha - \sigma^\alpha - \sum_k \nu_k^\alpha r^k = 0$$

$$R^{-1} = Y = \begin{bmatrix} D & S & 0 \\ S^T & 0 & 0 \\ 0 & 0 & K \end{bmatrix}$$

(Linear irreversible thermodynamics)

- D is P.D.
- Y has full rank

$$Y = \begin{bmatrix} D & S & 0 \\ S^T & 0 & 0 \\ 0 & 0 & K \end{bmatrix}$$

Euler-Lagrange equations:

$$\begin{bmatrix} j^\alpha \\ \sigma^\alpha \\ r^k \end{bmatrix} + Y \begin{bmatrix} -\nabla\lambda \\ -\lambda \\ -\nu^T\lambda \end{bmatrix} = 0$$

Role of strain balance (continuity), and couplings σ^α:

- "pV" work terms
- convections $\rho^\alpha \mathbf{v}$: $\Rightarrow J^\alpha = D\nabla\lambda$
- (External fields "g")

Elliptic system in adjoints (dual potentials)

EL + constraints:

$$\sum_\beta \left[\sum_{i,j} D_{ij}^{\alpha\beta} \frac{\partial^2}{\partial x_i \partial x_j} \lambda^\beta + \sum_i \left(S_i^{\alpha\beta} - S_i^{\beta\alpha} + \sum_j \frac{\partial D_{ij}^{\alpha\beta}}{\partial x_j} \right) \frac{\partial \lambda^\beta}{\partial x_i} - \left(k^{\alpha\beta} - \sum_i \frac{\partial S_i^{\alpha\beta}}{\partial x_i} \right) \lambda^\beta \right] = 0$$

Convex

B.C.:

$$\sum_\alpha B_{x,m}^\alpha \left(\sum_{\beta,i,j} n_i D_{ij}^{\alpha\beta} \frac{\partial \lambda^\beta}{\partial x_j} + S_i^{\alpha\beta} \lambda^\beta \right) = g_{x,m}$$

$$\sum_\alpha B_{\lambda,m}^\alpha \lambda^\alpha = g_{\lambda,m}$$

Field solution: Dual λ^α $\rightarrow$ E-L $\rightarrow$ Primal j^α, σ^α, r^k

Local equilibrium model

Extended thermodynamics

$$dS = \frac{1}{T} dE + \frac{\mathbf{P}\cdot\mathbf{F}^{-1}}{\rho T} : d(V\rho\mathbf{F}) - \sum_i \frac{(\mu^i + \phi^i)}{T} dN^i - \frac{\mathbf{v}}{T}\cdot d\mathbf{p} - \frac{M}{T} d\phi$$

$$\lambda^\alpha = \frac{\partial \sigma^S}{\partial \rho^\alpha}: \quad \begin{aligned} \lambda^i &= -\frac{(\mu^i + \phi^i)}{T} & \lambda^{\mathbf{p}} &= -\frac{\mathbf{v}}{T} \\ \lambda^{\mathsf{E}} &= \frac{1}{T} & \lambda^{\mathbf{F}} &= \frac{\mathbf{P}\cdot\mathbf{F}^{-1}}{\rho T} \end{aligned}$$

$\sigma^S(\rho^\alpha)$ convex (stable phases)

$\downarrow$

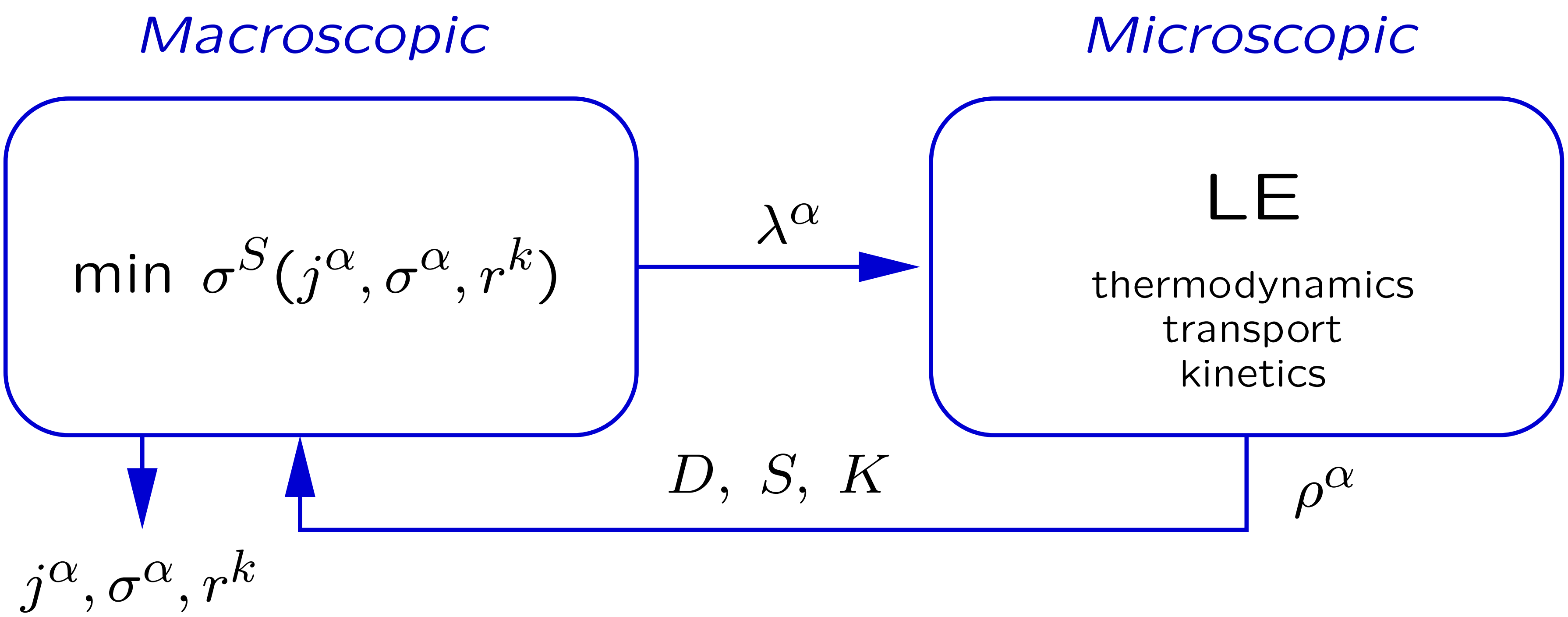
Point-to-point mapping

$\Downarrow$

Input $\lambda^\alpha \rightarrow \rho^\alpha \rightarrow$ Outputs D, K transport/kinetic resistances

$\rho^\alpha,\ \rho^\alpha\mathbf{v} \rightarrow S$ convection densities, couplings

Combined



Directional coupling

- Framework contains ∼all conventional phenomena
- Unified formulation - all submodels

Subsystems i: Integration over geometry to boundaries

Fixed frames in space

Basis fields:

$$\lambda \;=\; \sum \phi_q w_q \;=\; \Phi w\,, \qquad \nabla\lambda \;=\; \nabla\Phi w$$

$w \sim$ magnitude; character: flow directions, laminar/turbulent. . .

Integrations

$$\overline{\Phi}_{ij} \;=\; \iint_{A_{ij}} \Phi dA\,, \qquad \overline{\Phi}_i \;=\; \iiint_{V_i} \Phi dV \quad \text{etc.}$$

- Integrals evaluated empirically - friction factors, HT coefficients,. . .

Basis fields:

$$\lambda = \sum \phi_q w_q = \Phi w \,, \qquad \nabla\lambda = \nabla\Phi w$$

Integrations

$$\overline{\Phi}_{ij} = \iint_{A_{ij}} \Phi dA \,, \qquad \overline{\Phi}_i = \iiint_{V_i} \Phi dV \quad \text{etc.}$$

E-L + conservations

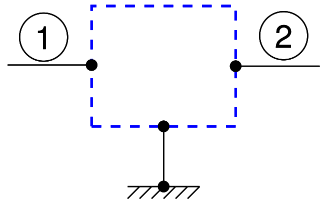
Flow at interface $i \to j$: $$x_{ij} = \iint_{A_{ij}} \mathbf{j} \cdot dA = (\overline{D}_{ij}\overline{\nabla\Phi}_{ij} + \overline{S}_{ij}\overline{\Phi}_{ij})w$$

$$\longrightarrow \quad \left[\sum_j (\overline{D}_{ij}\overline{\nabla\Phi}_{ij} + \overline{S}_{ij}\overline{\Phi}_{ij}) - \overline{S}_i^T \overline{\nabla\Phi}_i - \nu \overline{K}_i \nu^T \overline{\Phi}_i \right] w = 0$$

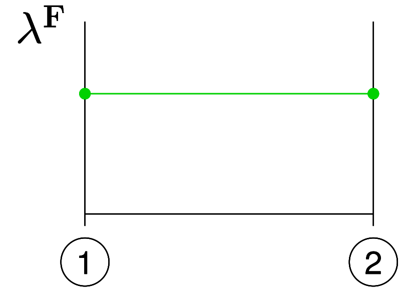
& BC's

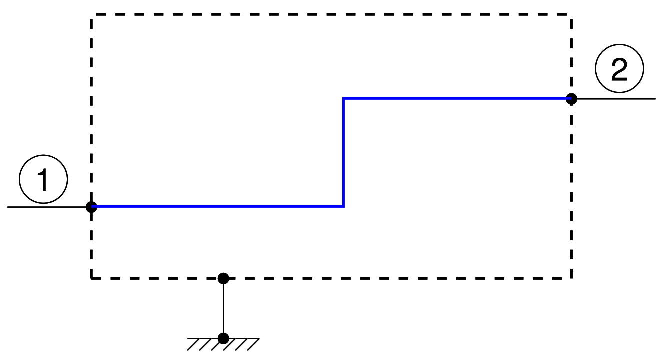
Examples: Piping Pattern

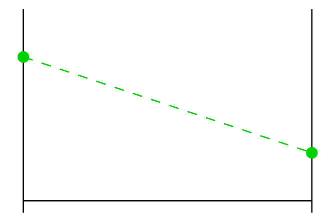
abstract



$$P_2 = P_1$$
$$(\mathbf{p}_2 \neq \mathbf{p}_1)$$
$$E_2 = E_1$$

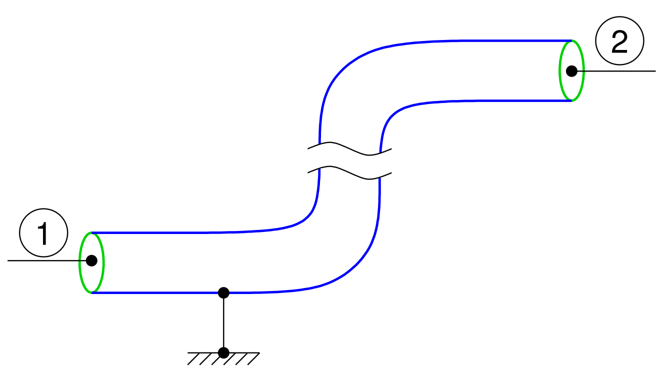


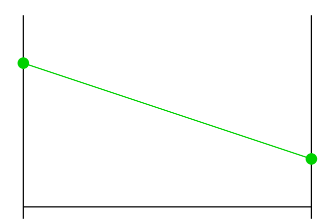




$$P_2 = P_1 - \Delta P_f - \rho g \Delta z$$

detailed

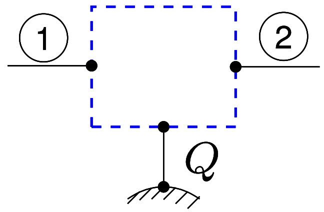




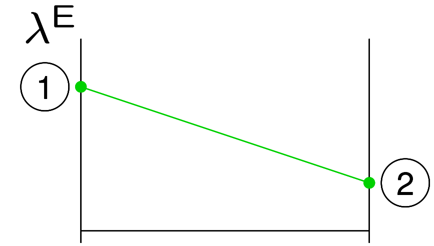
$$\Delta \left[\frac{v^2}{2} + \frac{P}{\rho} + gz \right]_1^2 + h_f = 0$$

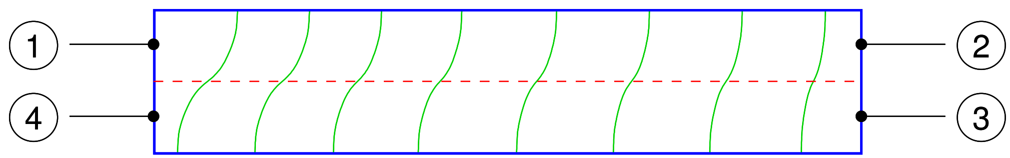
Examples: Heat Exchanger

abstract

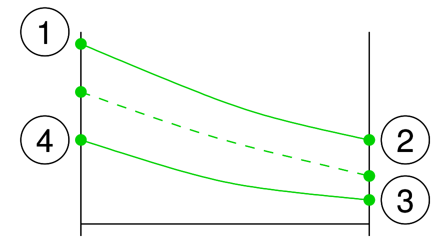


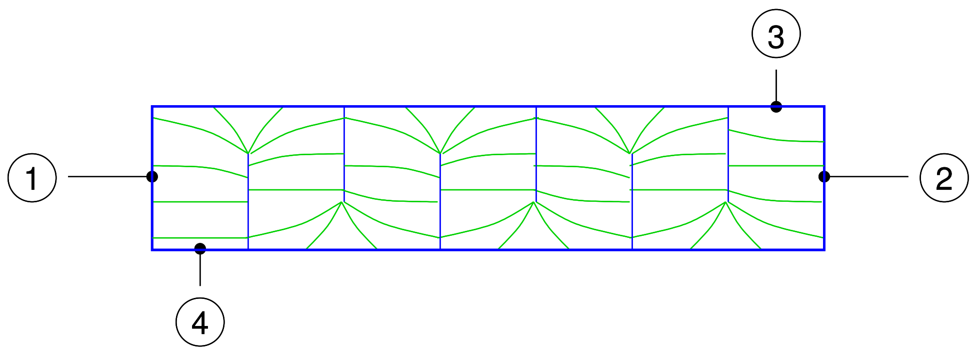
one-sided



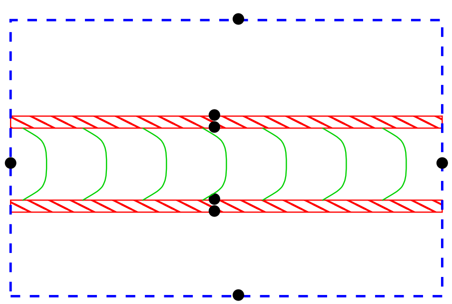


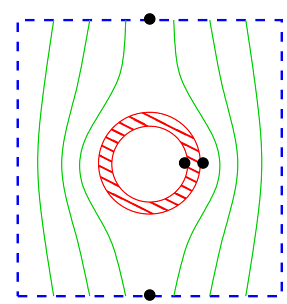
$$\Phi \quad \longleftrightarrow \quad \epsilon = \mathrm{fn}\left(N_{\mathrm{TU}}, \frac{(\dot{m}Cp)_1}{(\dot{m}Cp)_4} \right)$$





detailed

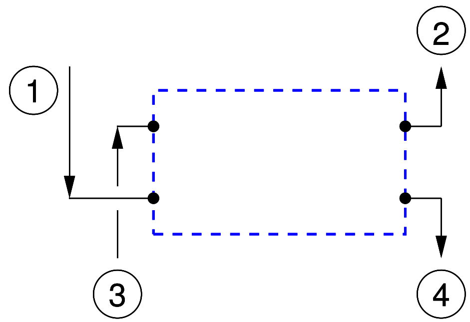




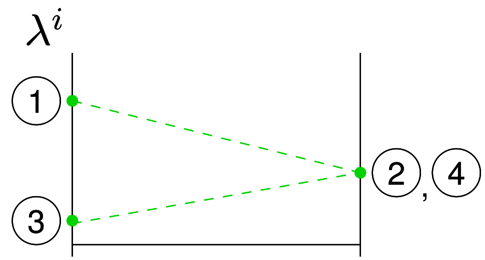
$$Q = hA\Delta\lambda^{\mathrm{E}}$$

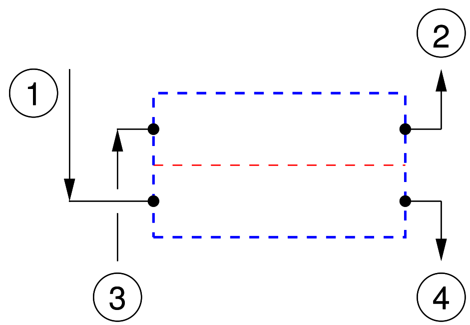
Examples: # Column Tray

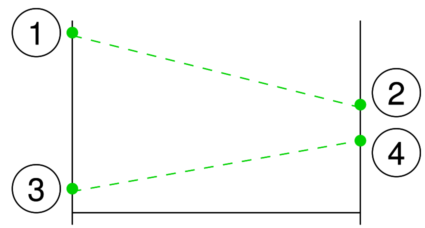
abstract



$$\lambda_2^i = \lambda_4^i$$

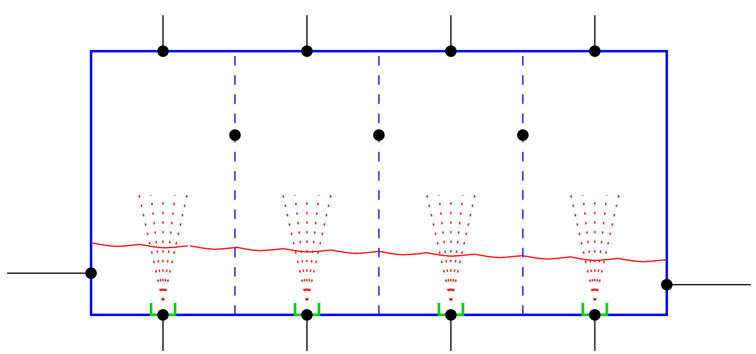




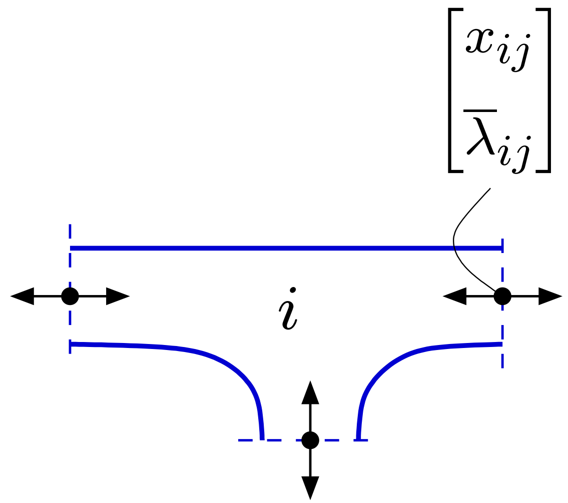


$$\lambda_2^i - \lambda_1^i = \sum_k E_{ik}^{\lambda,V} (\lambda_4^i - \lambda_1^i)$$

detailed



Subsystem BC's



Theorem:

Can specify either λ^α or $\nabla\lambda^\alpha$ at each point on boundary of domain of elliptic

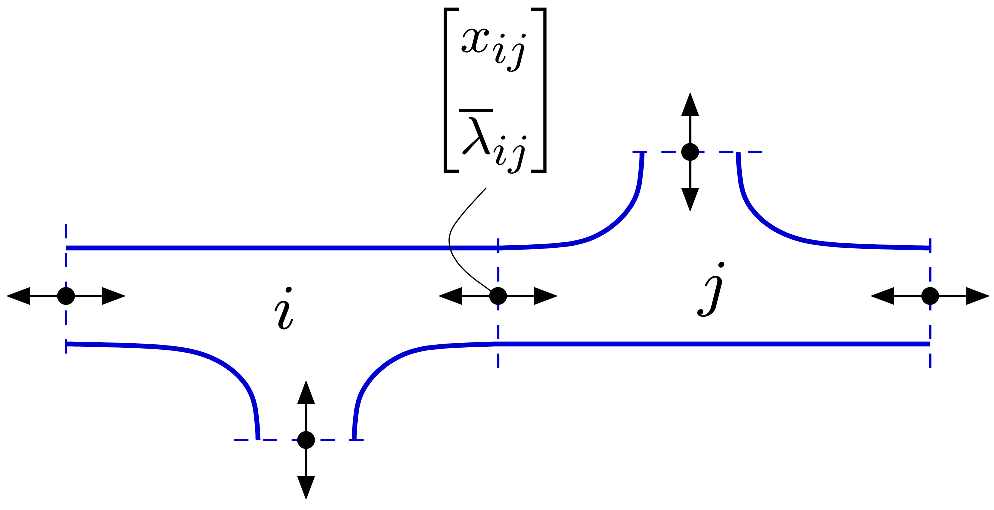
External boundary conditions

- Complementarity: specify either one of the pair

  (One per interface, each α)

$\hookrightarrow$ Rank requirement of basis fields: $\overline{\lambda}_{ij} = \frac{1}{A_{ij}} \overline{\Phi}_{ij} w_i \quad \text{rank} = \# j$

Subsystem combination into composite model



Connection → Internal boundary conditions

- Each pair $(x_{ij}^{\alpha}, \overline{\lambda}_{ij}^{\alpha})$ is *one* joint d.f.
- Equality between subsystems at interface jointly specifies the pair

$$\overline{\Phi}_{ij} w_i = \overline{\Phi}_{ji} w_j$$

linear conditions

& Remaining external boundary conditions

- One of complementary pair per interface, each α

Mappings

Interface $i \to j$:

Potential: $\overline{\lambda}_{ij} = \frac{1}{A_{ij}} \overline{\Phi}_{ij} w_i$

Flow: $x_{ij} = \iint_{A_{ij}} \mathbf{j} \cdot dA = (\overline{D}_{ij} \overline{\nabla\Phi}_{ij} + \overline{S}_{ij} \overline{\Phi}_{ij}) w_i$

E-L + conservations i:

$$\longrightarrow \quad \left[\sum_j (\overline{D}_{ij} \overline{\nabla\Phi}_{ij} + \overline{S}_{ij} \overline{\Phi}_{ij}) - \overline{S}_i^T \overline{\nabla\Phi}_i - \overline{K}_i \nu^T \overline{\Phi}_i \right] w_i = 0$$

Internal BC's:

$$\overline{\lambda}_{ij} - \overline{\lambda}_{ji} = \frac{1}{A_{ij}} \overline{\Phi}_{ij} w_i - \frac{1}{A_{ij}} \overline{\Phi}_{ji} w_j = 0$$

$$x_{ij} - x_{ji} = (\qquad) w_i - (\qquad) w_j = 0$$

External BC's:

$\overline{\lambda}_{ij} = \frac{1}{A_{ij}} \overline{\Phi}_{ij} w_i = \ldots$ or $x_{ij} = (\qquad) w_i = \ldots$

Aggregate all subsystems:

F^{field}:

$$w = \bigcup_i w_i$$

$$\bigcup_i \left(\left[\sum_j (\overline{D}_{ij} \overline{\nabla\Phi}_{ij} + \overline{S}_{ij} \overline{\Phi}_{ij}) - \overline{S}_i^T \overline{\nabla\Phi}_i - \overline{K}_i \nu^T \overline{\Phi}_i \right] w_i = 0 \right)$$

$$\downarrow$$

$$\overline{\lambda}_{ij} = \tfrac{1}{A_{ij}} \overline{\Phi}_{ij} w_i$$

$$\Downarrow$$

$$
\begin{array}{lll}
F_{ij}^{\text{LE}}: & \overline{\lambda}_{ij} & \longrightarrow \overline{D}_{ij}, \overline{S}_{ij}, \overline{K}_i \\
F^{\text{field}}: & \overline{D}_{ij}, \overline{S}_{ij}, \overline{K}_i \longrightarrow w \longrightarrow \lambda & \longrightarrow \overline{\lambda}_{ij} \\
 & & \longrightarrow \overline{j}_{ij}, \overline{\sigma}_i, \overline{r}_i \\
 & & \longrightarrow x_{ij}
\end{array}
$$

Solution of composite model via homotopy

Composed mapping:

$$\begin{bmatrix} x_{ij} \\ \overline{\lambda}_{ij} \end{bmatrix} = F_{ij}(\,\overline{\lambda}_{ij}\,) = F_i^{\text{field}}\big(\,F^{\text{LE}}(\,\overline{\lambda}_{ij}\,)\,\big)$$

- Identify $\overline{\lambda}_{ij}$ $(\,=\,\overline{\lambda}_{ji}\,)$
- Initial $\overline{\lambda}^{0}_{ij}$, w^0
  - External specifications; other d.f. arbitrary
  - Feasibility validation by linear algebra
- Homotopy:

$$H_{ij}(t, \overline{\lambda}_{ij}, \cdot) = \left(F_{ij}(\,\overline{\lambda}_{ij}\,) - F_{ji}(\,\overline{\lambda}_{ij}\,)\right) - \left(F_{ij}(\,\overline{\lambda}^{0}_{ij}\,) \;-\; F_{ji}(\,\overline{\lambda}^{0}_{ij}\,)\right)(1-t)$$
$$= (x_{ij} - x_{ji}) \;-\; (x^0_{ij} - x^0_{ji})(1-t) \;=\; 0$$

- Always dual-feasible, converge primal flows

Proofs

Theorem 1

Convexity by 2nd Law plus BC rank from complementarity:

F^{field}: **Elliptic field solution exists and is unique**

Theorem 2

Convexity by thermodynamic stability

F^{LE}: LE gives an unique point mapping

Theorem 3

(Kakutani-Glicksburg-Fan)

Domain of map($\overline{\lambda}$) is convex, compact

Range of F is in domain

Composite coupled solution exists

Result:

Homotopy path points exist and remain bounded

$\longrightarrow$ Path will converge to a solution.

(Multiple solutions are possible)

Capabilities Enabled

- Global convergence – generic initial point
- Interface compatibility – canonical $\longrightarrow$ universal

  model refinement / abstraction submodels independently

  nested structures of submodels
- Incorporation of the engineering knowledge base

  dimensionless correlations

  automatic, consistent property averaging
- D.F. specification – validation

Ongoing...

Better appreciation of "geometry"	Time
Symmetries	Optimization

Acknowledgments

C.A. Amundson

UW sabbatical program

Ignacio Grossmann