Exergy Based Methods for Multidisciplinary Analysis & Design

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Program

- Multidisciplinary Science & Technology Center
- Entropy & 2nd Law
- Concept of Exergy
- Case Studies

AFRL Air Vehicles In-House Research Centers

MULTIDISCIPLINARY SCIENCE & TECHNOLOGY

★Center Goals

- *Bring system-level interdisciplinary interactions earlier in the design process*
- *Bring appropriate level of fidelity across all stages of the design process: Conceptual → Preliminary → Detailed*
- *Capture and model RELEVANT PHYSICS before flight*
- *Complement with experimentation to validate the science*

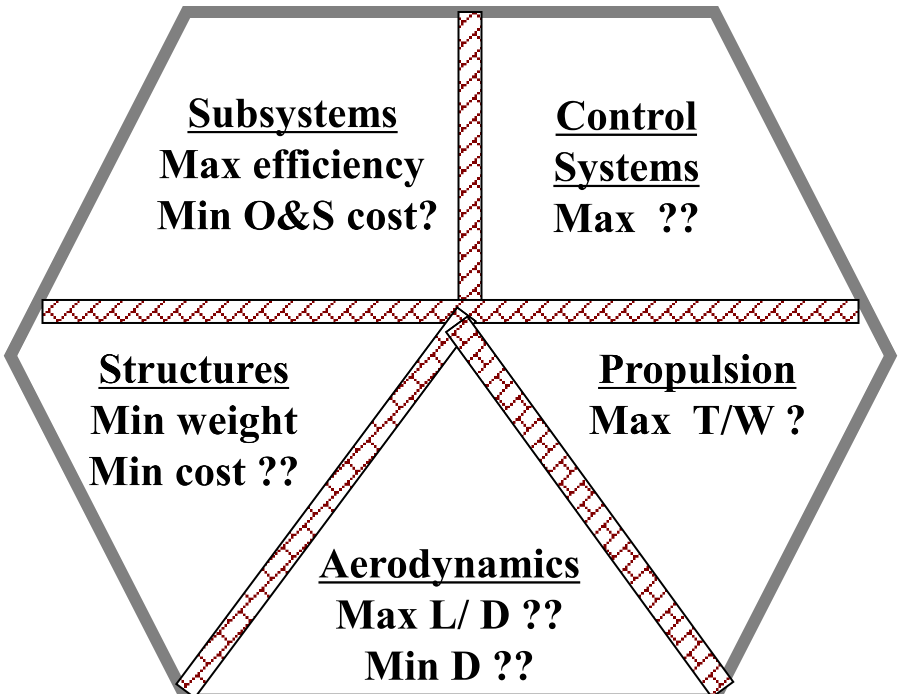
Why Multidisciplinary?

- ★ Systems are Becoming More and More Integrated
- ★ Technology (Disciplinary) Interactions can be First-Order Effects
- ★ Effects Can be Beneficial or Adverse
- ★ Single-Discipline or Component Optimization Gives a Sub-Optimum Overall System

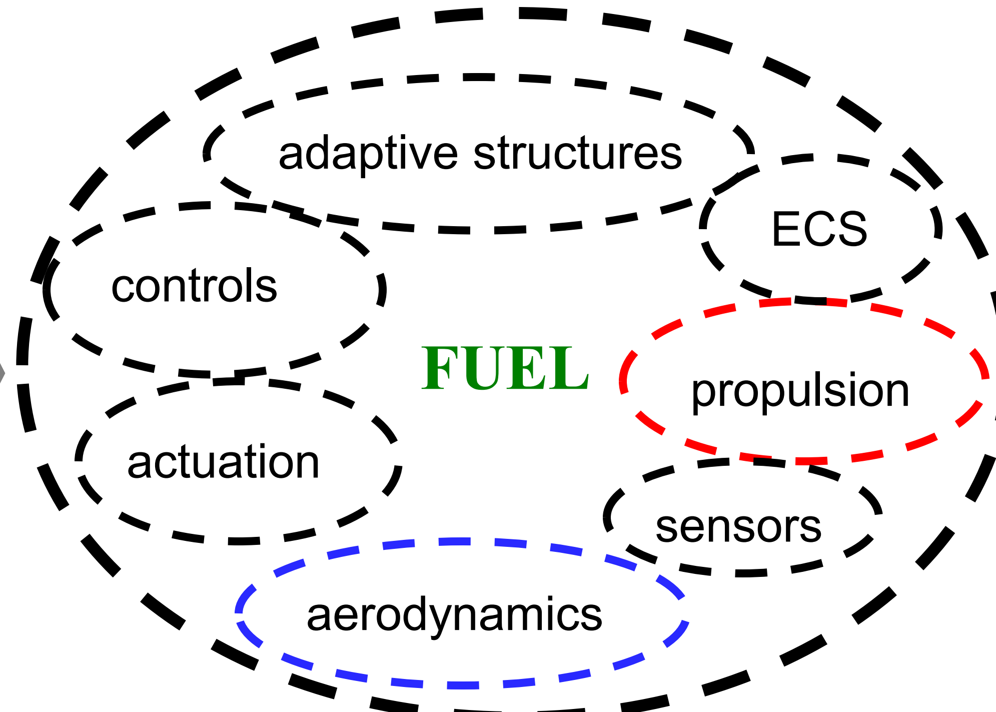
Total System Optimization for Energy Efficient Vehicles

The Multidisciplinary Problem & Solution

TRADITIONAL DEVELOPMENT OF INDIVIDUAL COMPONENTS, THEN PLUG THEM TOGETHER



TRUE
SYSTEM OPTIMIZATION
must be *WHOLISTIC*



Fundamental Challenge: How to integrate performance metrics across multiple disciplines?

Scientific & Technical Challenge

- **How to integrate, e.g., propulsion system and aerodynamics?**
  - *Performance metrics different: L /D, etc for aerodynamics; various engine efficiencies for propulsion systems.*
- **Fundamental challenge:**
  - *Find a uniform way to trade performance metrics across multiple disciplines, systems, and scales.*
  - *Need a universal property that quantifies performance.*
  - *Candidates:*
    - Energy is a universal property → First Law of Thermodynamics
    - Entropy is a universal property → Second Law of Thermodynamics
    - Both recognized as important in all natural processes, including physics-based, engineering machines. Is a synthesis of the two available?

YES! Exergy ←→ Work Potential

Second Law Interlude

ENTROPY MYSTIQUE

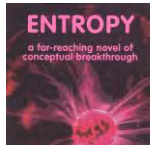
On Thermodynamics

"Thermodynamics is a funny subject.

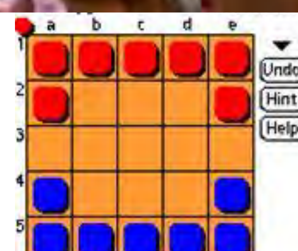
- *The first time you go through it, you don't understand it at all.*
- *The second time you go through it, you think you understand it, except for one or two small points.*
- *The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you any more."*

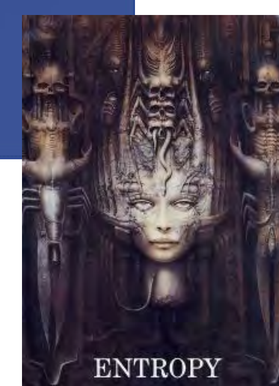
– *Arnold Sommerfield.*

Entropy is…




- ★ Order
- ★ Disorde
- ★ Chaos
- ★ Informa
- ★ A heavy
- ★ A “happ
- ★ Tanning
- ★ Floor co
- ★ A “semi
- ★ Ticket Dispenser
- ★ The list goes on!



On the One Hand…

Quote from popular undergraduate text book:

"Finally, the second law of thermodynamics relates entropy change dS to heat added dQ and absolute temperature T

$$dS \geq {dQ}/{T}$$

This is valid for a system and can be written in control-volume form, *but there are almost no practical applications in fluid mechanics <u>except to analyze flow-loss details</u>.*"

Fluid Mechanics by F. M. White, McGraw-Hill (1979), pp. 125.

On the Other Hand…

- ★ The law that entropy always increases—the second law of thermodynamics—holds, I think, the supreme position among the laws of Nature.
- ★ If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equations—then so much the worse for Maxwell's equations.
- ★ If it is found to be contradicted by observation, well, these experimentalists do bungle things sometimes.
- ★ *But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation.*

—A. S. Eddington, 1948.

The Basic Concept

EXERGY

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Classical Thermodynamics

- **First Law: There exists a quantity called energy which behaves like a fluid-like substance that is conserved.**
  - *Principle of energy conservation*
- **Second Law: There exists a quantity called entropy which behaves like a fluid-like substance that is never destroyed in any natural process.**
  - *Principle of non-negative entropy generation; maximum entropy.*
  - *Maximum possible efficiency for any heat engine.*
  - *Maximum possible work extraction for any cyclic process; Clasius-Duhem inequality, Kelvin-Planck statement, Carnot cycle, etc.*

Laws of Thermodynamics

★ **First Law:** *Energy is a state property.*

$$\dot{E}_{in} - \dot{E}_{out} = \dot{E}_{\Omega}$$

★ **Second Law:** *Entropy is a state property.*

$$\dot{S}_{\mathrm{in}} - \dot{S}_{\mathrm{out}} + \dot{S}_{\mathrm{gen}} = \dot{S}_{\Omega}$$

★ **Principle of Non-negative Entropy Generation:**

$$\dot{S}_{\mathrm{gen}} \geq 0$$

The Second Law in Classical Thermodynamics

- **Entropy:**

$$S = S(U)$$

- **Second Law:**

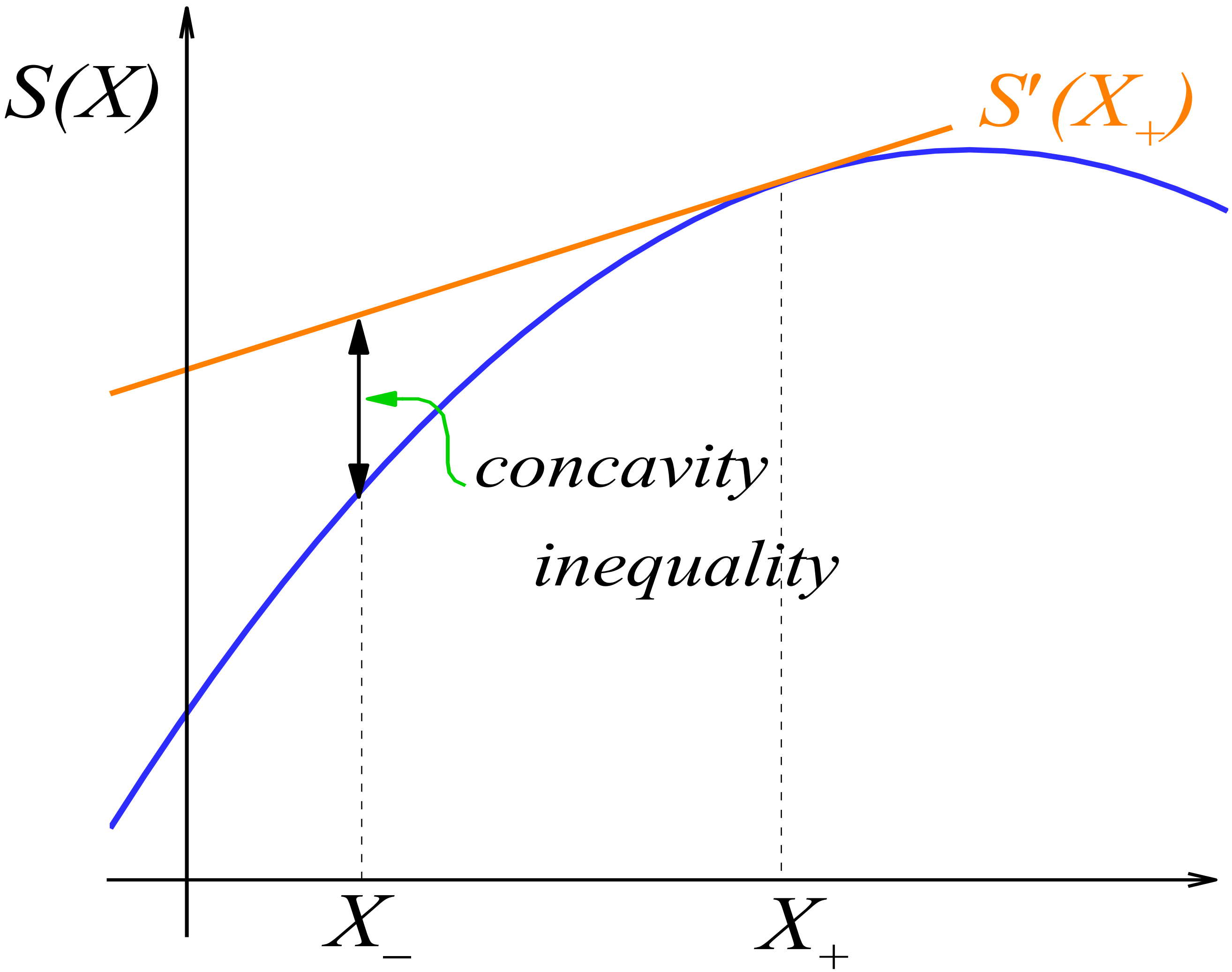
$$\int_{t}^{t_0} \dot{S}_{\text{gen}} dt = S_0 - S - \left.\frac{\partial S}{\partial U}\right|_0 (U_0 - U)$$

- **Concavity:**

$$S_0 - S - \left.\frac{\partial S}{\partial U}\right|_0 (U_0 - U) \geq 0$$

Entropy Concavity

$$S(X_+) - S(X_-) - S'(X_+)(X_+ - X_-) \geq 0$$



Concept of Exergy

- **Conventional Approach:**
  - *Introduce "availability" or "exergy" in context of "system potential to perform work in a reversible manner".*
  - *Multiple work terms introduced: reversible work, available work, useful work, etc.*
  - *Leads to confusion and cluttering in terminology.*
- **Revised Approach:**
  - *Utilize the essence of the second-law by interpreting exergy as an abstract thermodynamic metric.*
  - *Exergy quantifies the "distance" from arbitrary initial state to state of equilibrium with reference conditions.*
  - *Theoretical limits of engineering devices utilizing thermophysical processes provided by "second-law efficiency" or effectiveness.*

Thermo-101 Derivation of Balance of Exergy

★ **Energy:**

$$E_0 - E = Q_0 - W_0$$

★ **Entropy:** $$T_0\left(S_0 - S\right) = Q_0$$

★ **Mechanical Energy Transfer:**

$$W_0 = \int PdV = W_{\mathrm{useful}} + P_0\left(V_0 - V\right)$$

Mathematical Definition of Exergy

- **Useful work potential:**

$$W_{\text{useful}} = f\left(\underbrace{E, S, \ldots}_{\text{current state}} \middle| \underbrace{E_0, S_0, \ldots}_{\text{equilibrium with reference}}\right)$$

- **Exergy →** $X \equiv W_{\text{useful}}$

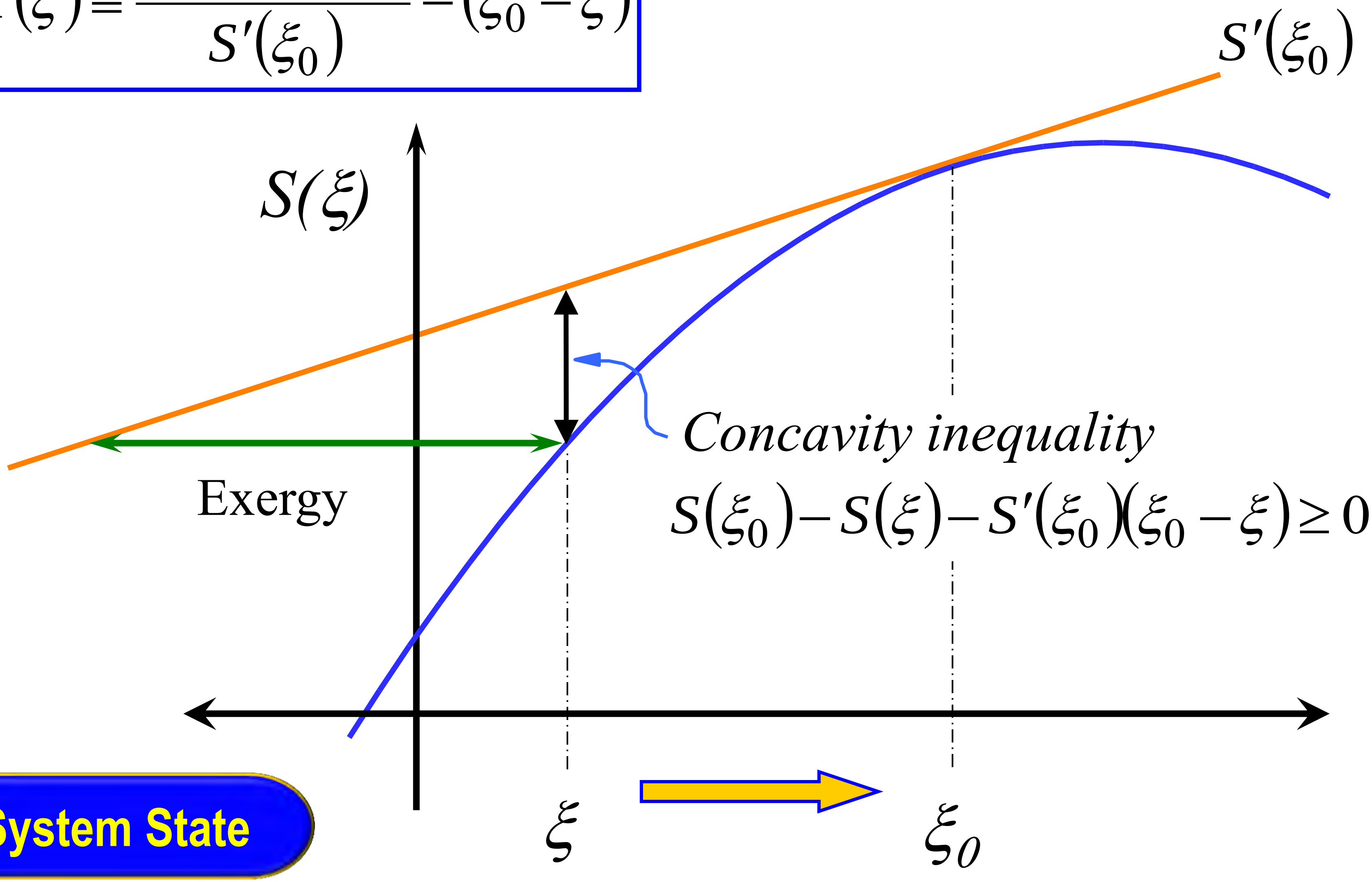
- **Construction of balance equation**
  - *First Law* → $\mathcal{L}_1$
  - *Second Law* → $\mathcal{L}_2$

$$\mathcal{L}_1 - T_0 \mathcal{L}_2$$

Camberos, J., "Revised interpretation of work potential in thermophysical processes," *AIAA J. Thermophysics & Heat Transfer*, **14**:2, p 177-185 (2000).

Exergy: Measures Distance to Equilibrium with Environment

$$X(\xi) \equiv \frac{S(\xi_0) - S(\xi)}{S'(\xi_0)} - (\xi_0 - \xi)$$



Measures of Performance

- **Balance of Exergy:**

$$\dot{X}_{\text{in}} - \dot{X}_{\text{out}} - T_0 \dot{S}_{\text{gen}} = \dot{X}_{\Omega}$$

- **Principle of Non-negative Entropy Generation**

$$T_0 \dot{S}_{\text{gen}} \geq 0$$

- **Second-Law Efficiency or Effectiveness**

$$\eta_{II} \equiv 1 - \frac{\dot{X}_{\text{destroyed}}}{\dot{X}_{\text{supplied}}}$$

Conventional MDA/MDO

- **Conventional MDO uses gradients (a.k.a., sensitivities).**
- **These coefficients are typically *normalized according to local variable dimensions* (e.g., fractional differences).**
  - *Cannot account for essential differences between aerodynamics (wing) and thermodynamics (engine).*
  - *Will not account for global changes.*
  - *Magnitude of sensitivities can mislead direction of optimization.*

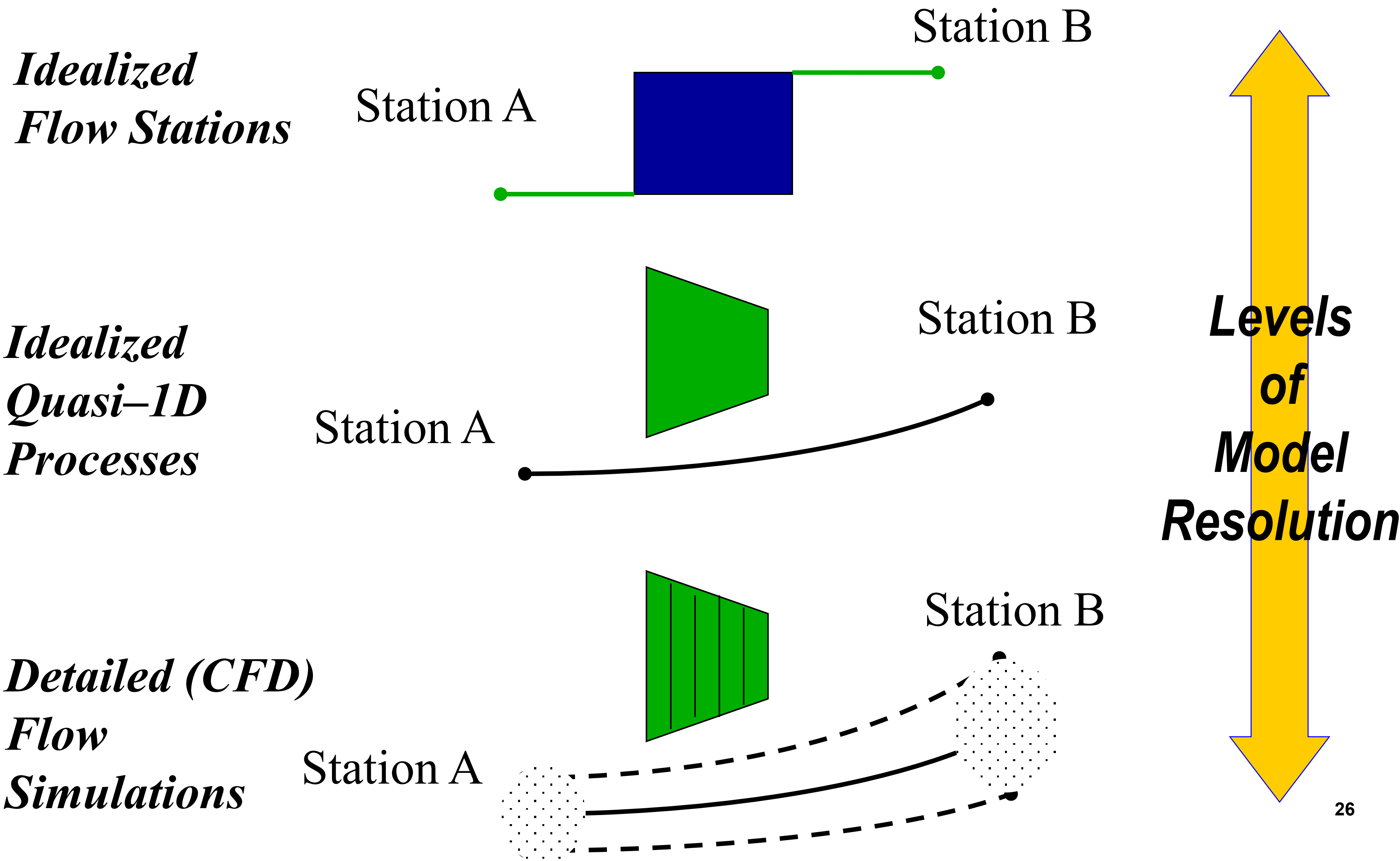
Exergy Based MDA/MDO

- **With true "common currency" as objective function:**
  - *Sensitivities are normalized according to global dimensions.*
  - *The magnitude of these sensitivities will be a better indication as to best direction for system optimization.*
  - *Provide a clear picture of total system integration.*
- **Will exclude (physically) infeasible directions.**
- **Will lead to areas of the design space that are excluded by conventional design methods/knowledge.**
  - *Opens viable possibilities for revolutionary design.*
- ***Minimum exergy-destruction will result in optimum performance, period.***

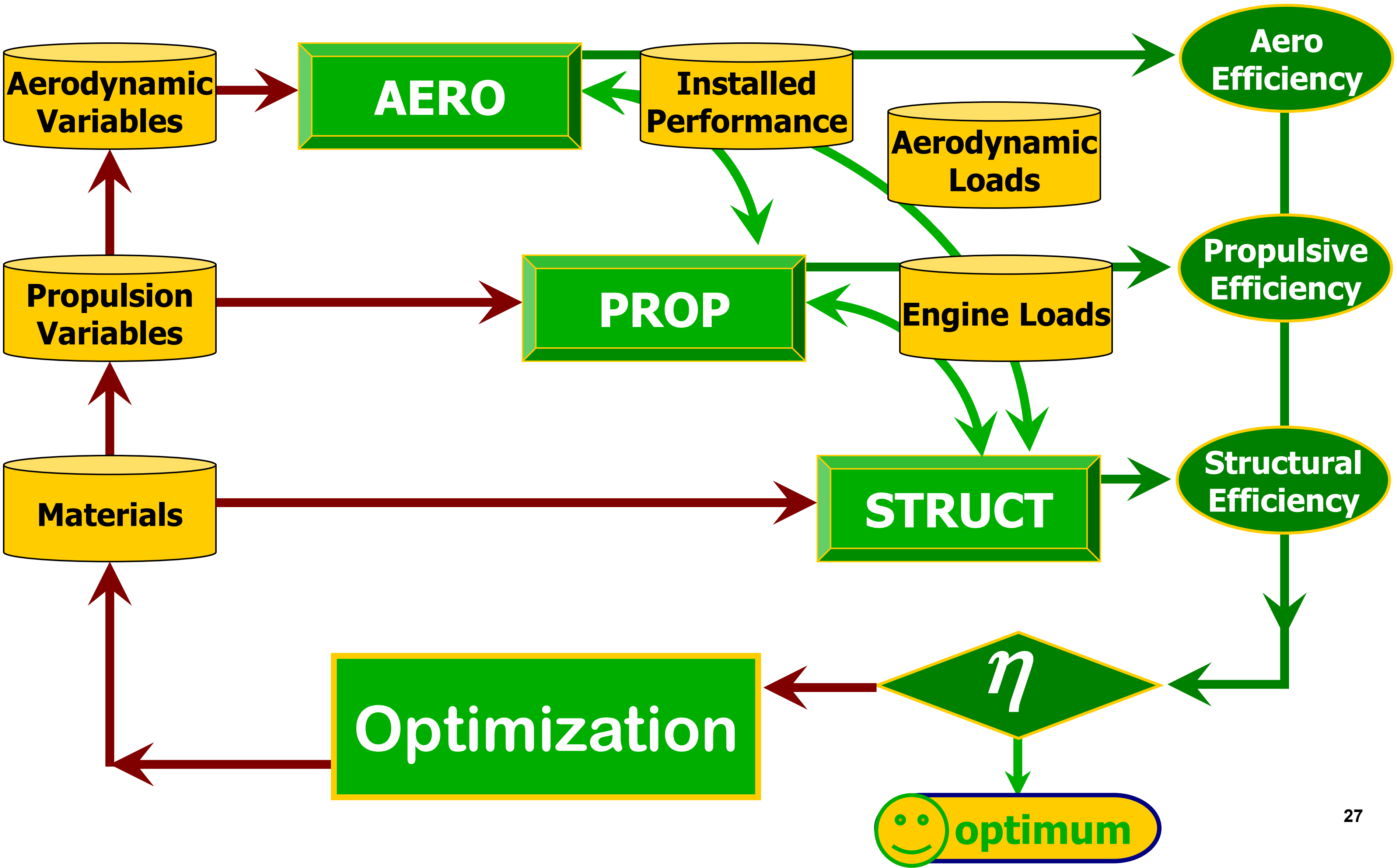
Payoff & Benefits

- **Thesis**
  - *Strongly integrated design process will yield better results in less time than conventional, weakly integrated, "over-the-wall", iterative trade-study.*
  - *Will enable new, revolutionary technology development, possibly lower cost.*
- **Systems engineering capability for truly integrating vehicle analysis & design.**
  - *Theoretical basis for analysis and design framework, offering the potential to perform conceptual design across multiple disciplines, scales, and levels of fidelity.*

Exergy Method Works Across Multiple Levels of Model "Resolution"



Multidisciplinary System Design



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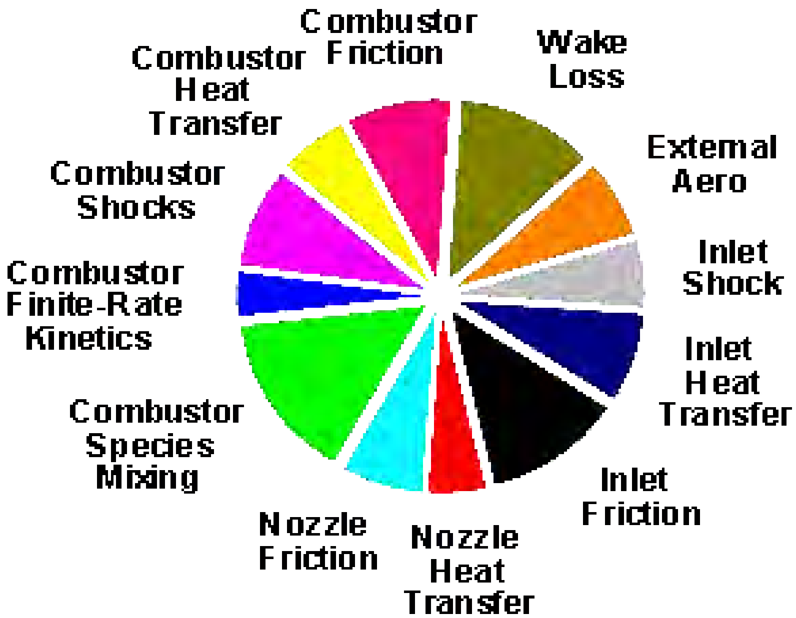
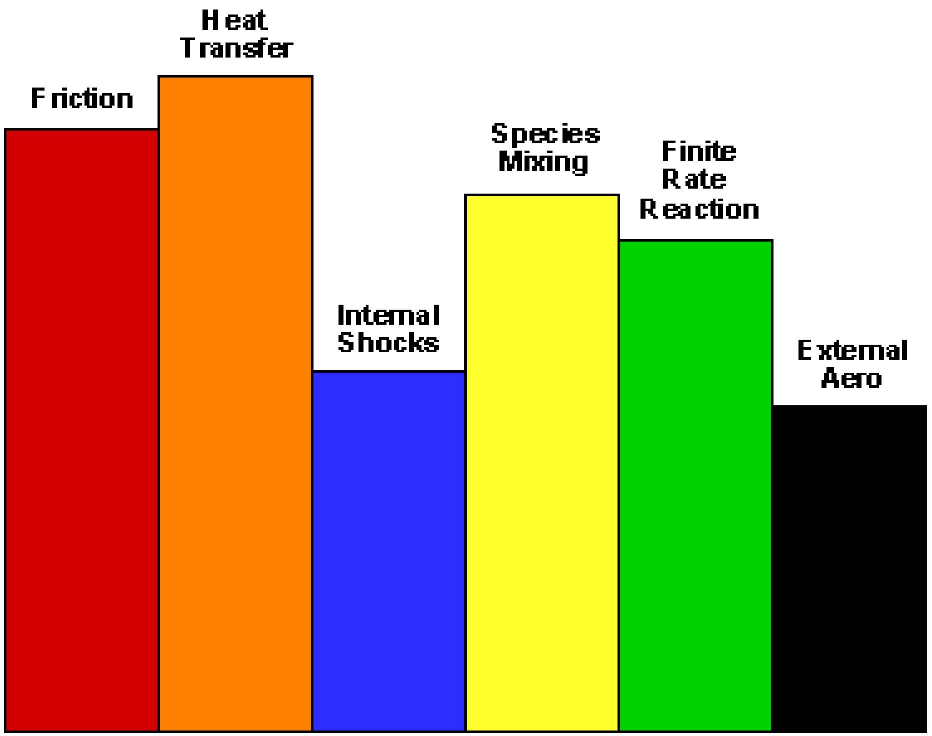
The Second Law

CASE STUDIES

Performance Audit

Vehicle Component





Physics

Aerodynamic Performance

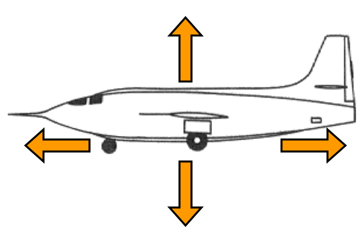
★ **Conventional (Force)**

- *Lift, drag, lift/drag, etc.*
  - Coefficients:

$$C_L = \frac{L}{\frac{1}{2}\gamma P M^2 A},$$

$$C_D = \frac{D}{\frac{1}{2}\gamma P M^2 A},$$

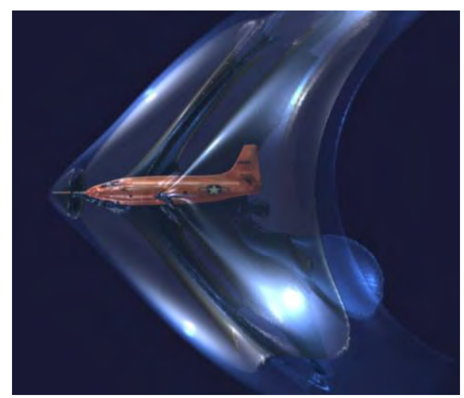
$C_{L,D}$ based on vehicle force balance.



★ **Unified (Exergy)**

- *Exergy Destruction*
  - Coefficient:

$$C_X = \frac{\rho T_0 \dot{S}_{gen}}{\gamma P M^2}$$

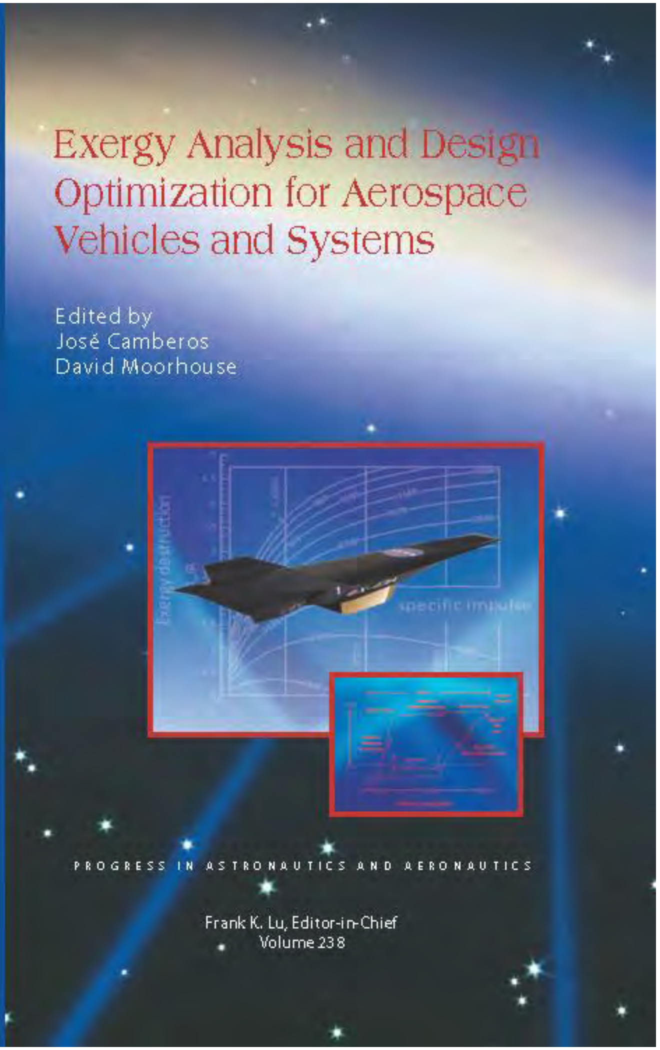


C_X is based on flowfield energetics.

Collaborators

- ★ Dr. Adrian Bejan, Duke University
- ★ Dr. John Doty, University of Dayton
- ★ Dr. Richard Figliola, Clemson University
- ★ Dr. Greg Naterer, University of Manitoba, Canada
- ★ Dr. Dave Riggins, University of Missouri-Rolla
- ★ Dr. Michael von Spakovsky, Virginia Tech

Reference



Preface – *Col. John Wissler*; Foreword – *Dr. Tom Curran*

1. Introduction – *Moorhouse*
2. Fundamentals of Exergy Analysis – *Camberos & Doty*
3. The Role of Exergy in System Analysis – *Doty & Camberos*
4. Integrated Subsystem Analysis Using Entropy-Generation Minimization– *Figliola*
5. Subsonic Aerodynamic Analysis Using Entropy-Generation Minimization with High-Fidelity Methods – *Figliola*
6. Entropy Generation & Aerospace Vehicle Perf. – *Riggins*
7. Optimization of High-Speed Aerospace Vehicles Using Entropy-Generation Minimization – *Riggins*
8. Theory and Examples of Mission Analysis Using Entropy Generation Analysis – *Riggins*
9. Mission Integrated Synthesis/Design Optimization (MIS/DO) of Aerospace Vehicles – *von Spakovsky*
10. MIS/DO Applied to High Speed, High Performance Vehicles – *von Spakovsky*
11. Thermodynamics, Entropy-Generation Minimization, and the Constructal Law – *Bejan*
12. Quantum Thermodynamics & Modeling of Non-equilibrium Phenomena: Theory and Future Directions – *von Spakovsky*
13. Numerical Methods in Light of the Second Law – *Camberos*

AIAA Progress in Astronautics & Aeronautics, 2011

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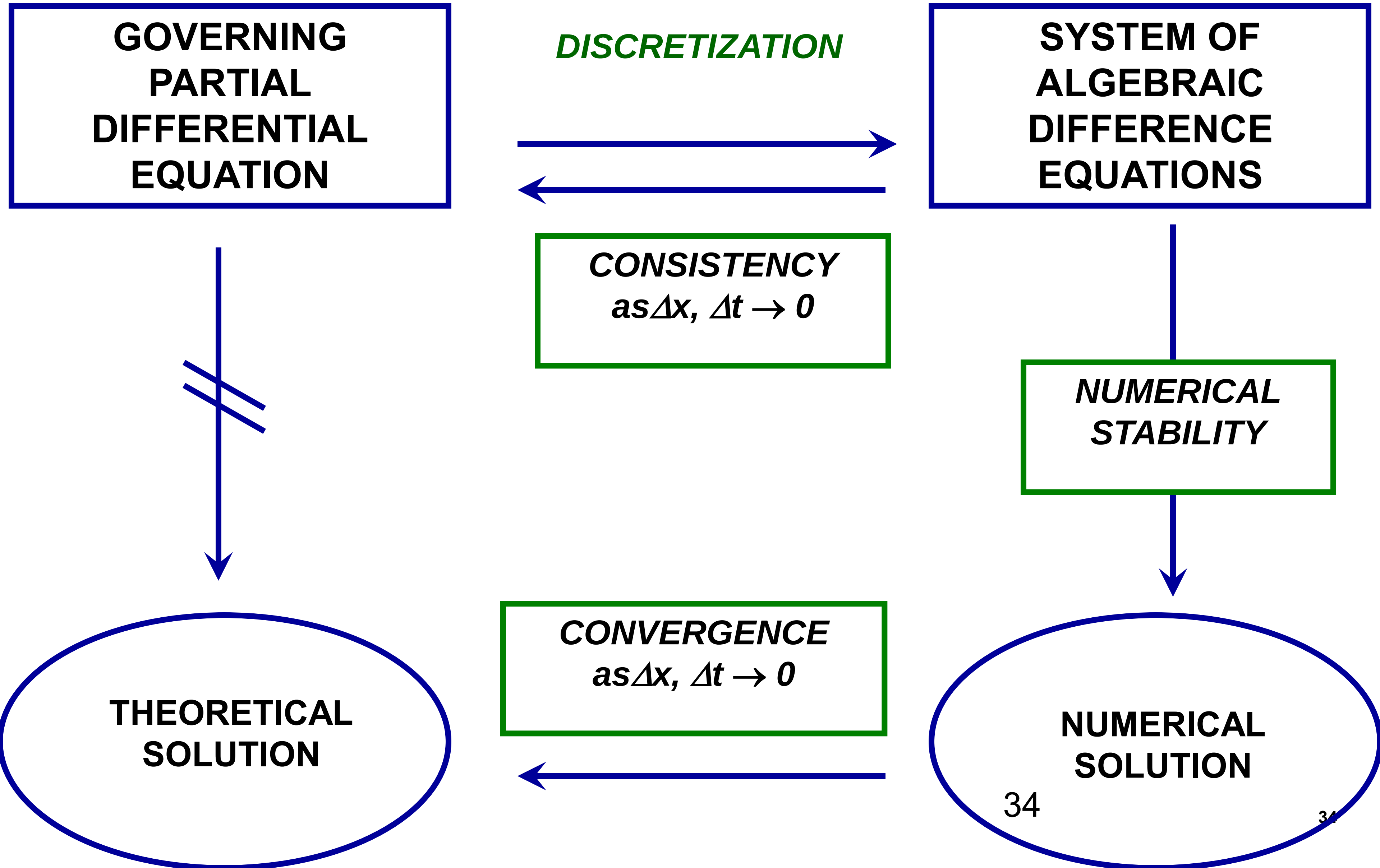
In Light of the Second Law

NUMERICAL METHODS

Properties of Numerical Solution



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SLT for the Global Domain

- **Essence of the second law is concavity.**

$$S(\bar{\boldsymbol{q}})-S(\boldsymbol{q})-\frac{\partial S}{\partial \bar{\boldsymbol{q}}}\cdot(\bar{\boldsymbol{q}}-\boldsymbol{q})\geq 0$$

- **Equality holds *iff***

$$\boldsymbol{q}=\bar{\boldsymbol{q}}\equiv\int_{\Omega}\boldsymbol{q}\,d\Omega\Big/\int_{\Omega}d\Omega=\langle\boldsymbol{q}\rangle$$

- **Averaging gives:**

$$\langle S(\bar{\boldsymbol{q}})-S(\boldsymbol{q})\rangle\geq 0$$

Construction of Error Metrics

- Near equilibrium, deviations from the average (mean) state are small. So approximate:

$$S(\bar{q}) - S(q) - S_{,\bar{q}} \cdot (\bar{q} - q) \approx -\tfrac{1}{2}(\bar{q} - q)^T \cdot S_{,\bar{q}\bar{q}} \cdot (\bar{q} - q)$$

- Mean-square variations measured by the norm

$$\|q\|^2 \equiv \left\langle q^T \cdot \left[-S_{,\bar{q}\bar{q}}\right] \cdot q \right\rangle$$

  - *Average entropy difference:* $\left\langle S(\bar{q}) - S(q) \right\rangle \geq 0$
  - *MSV relative to mean:* $\|q - \bar{q}\|^2 \geq 0$

Stability Implications of SLT

★ **Expand MSV relative to mean**

$$\|\boldsymbol{q}-\overline{\boldsymbol{q}}\|^2 = \|\boldsymbol{q}\|^2 - \|\overline{\boldsymbol{q}}\|^2$$

★ **From TSE near equilibrium,**

$$2\langle S(\overline{\boldsymbol{q}}) - S(\boldsymbol{q})\rangle + \|\overline{\boldsymbol{q}}\|^2 \approx \|\boldsymbol{q}\|^2$$

★ **Conjecture:**

$$\exists K_0 = K(\boldsymbol{q}_0) \ni$$

$$2\langle S(\overline{\boldsymbol{q}}) - S(\boldsymbol{q})\rangle + \|\overline{\boldsymbol{q}}\|^2 \geq K_0 \|\boldsymbol{q}\|^2$$

Stability Implications of SLT

- **Scaling constant determined from initial conditions.**

$$K_0 = \frac{2\langle \Delta S \rangle + \|\bar{\boldsymbol{q}}\|^2}{\|\boldsymbol{q}_0\|^2}$$

- **If SLT satisfied locally, then also satisfied globally:**

$$\langle S(\bar{\boldsymbol{q}}) - S(\boldsymbol{q}) \rangle \geq \langle S(\bar{\boldsymbol{q}}) - S(\boldsymbol{q}_0) \rangle \geq 0$$

- **Statement of Numerical Stability**

$$2\langle \Delta S_0 \rangle + \|\bar{\boldsymbol{q}}\|^2 \geq 2\langle \Delta S \rangle + \|\bar{\boldsymbol{q}}\|^2 \gtrsim K_0 \|\boldsymbol{q}\|^2 \geq 0$$

Numerical Experiments

★ Acoustic Wave Propagation.

- *Initial conditions*

$$\rho = \begin{cases} 1.0 & 0.00 \le \xi < 0.45 \\ 1.5 & 0.45 \le \xi \le 0.55 \\ 1.0 & 0.55 < \xi \le 1.00 \end{cases} \qquad \left.\begin{array}{l} u = 0 \\ T = 1 \end{array}\right\} 0 \le \xi \le 1.0$$

★ Shock Tube Simulation.

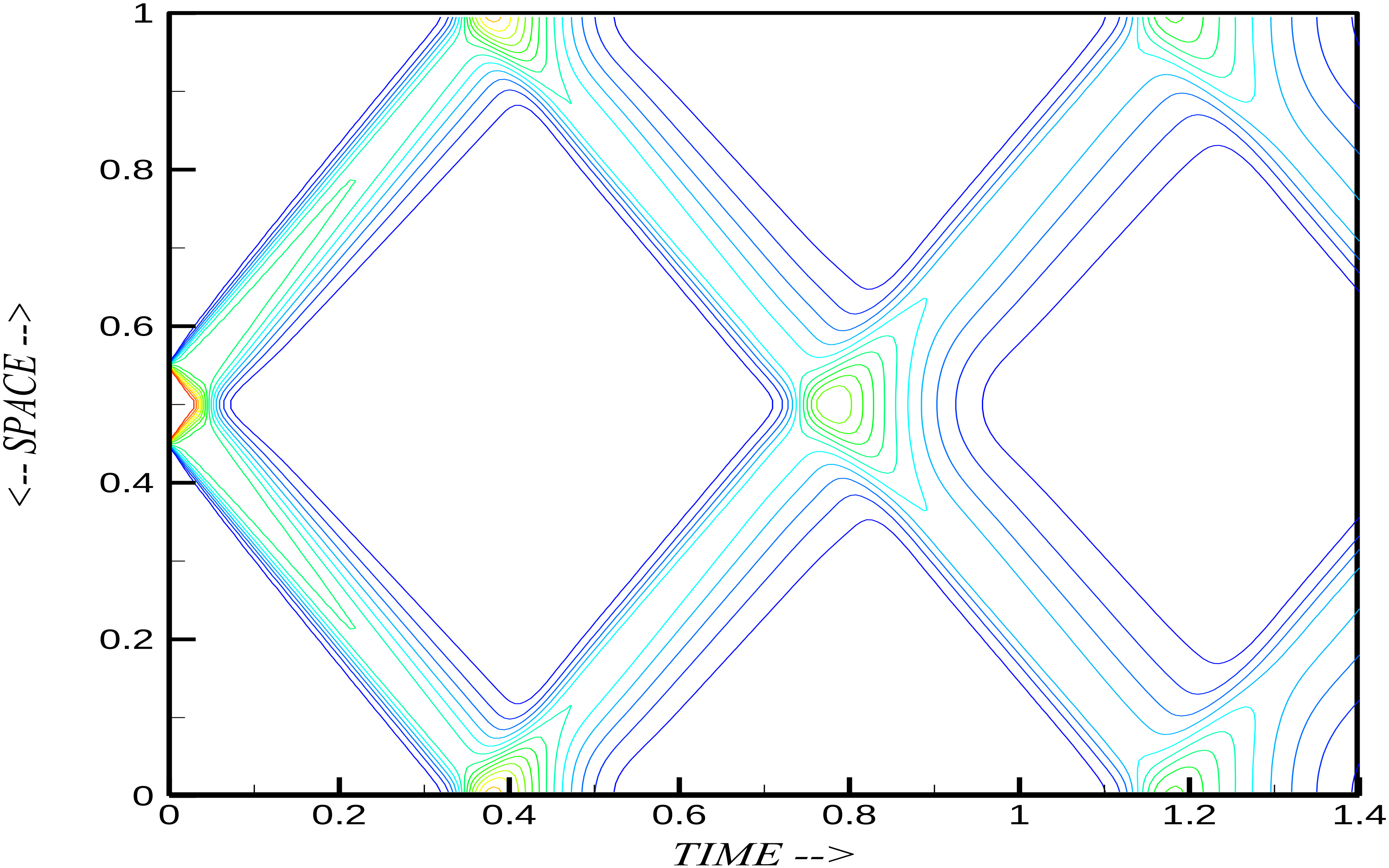
- *Initial conditions*

$$\left.\begin{array}{l} \rho = 1 \\ u = 0 \\ p = 1 \end{array}\right\} 0 \le \xi \le 0.5 \qquad \left.\begin{array}{l} \rho = 5 \\ u = 0 \\ p = 5 \end{array}\right\} 0.5 < \xi \le 1.0$$

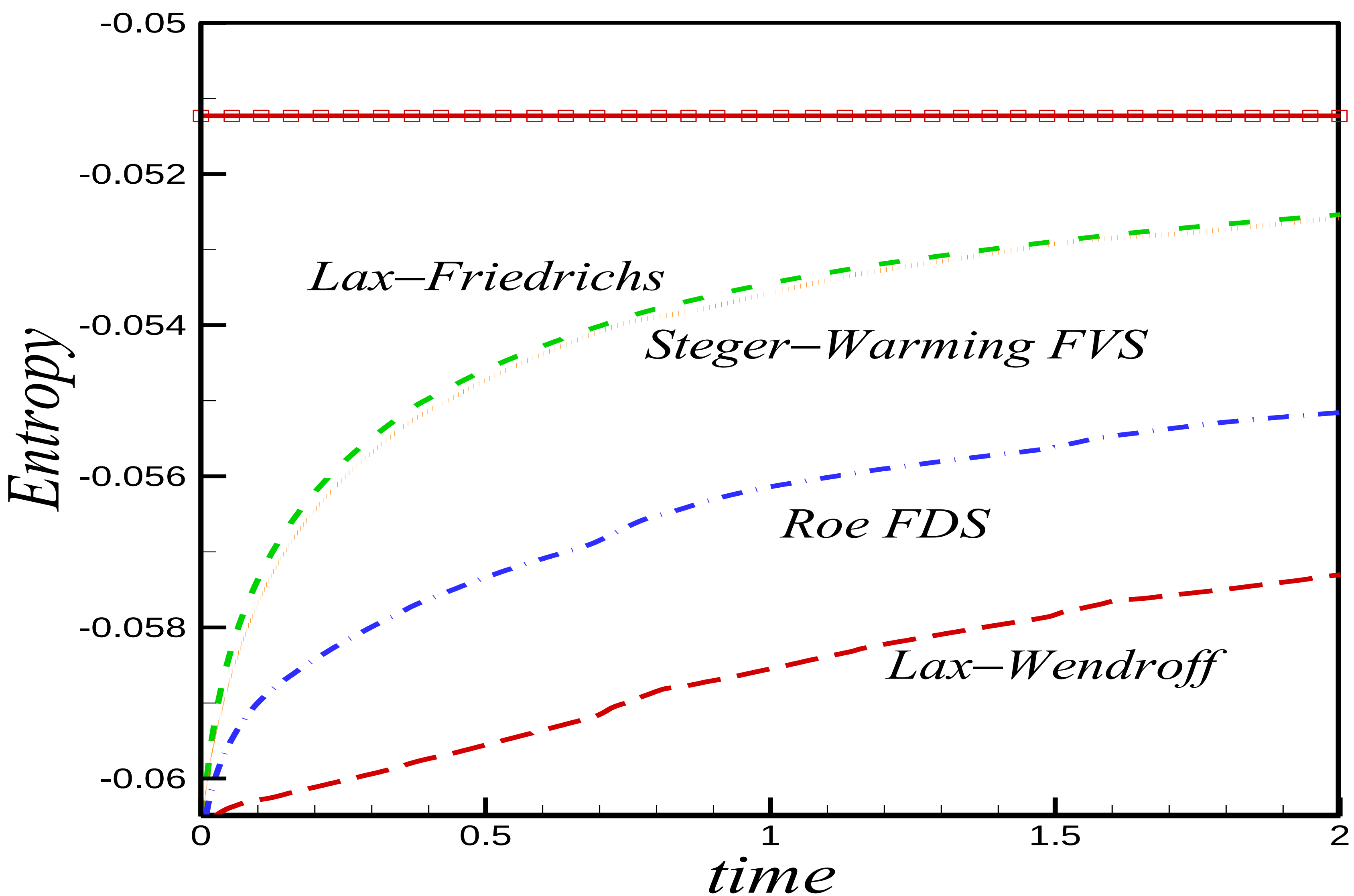
★ 1D Shock Structure Solution.

- *Rankine-Hugoniot initial conditions and boundary conditions held fixed, Mach number equal to 1.5*

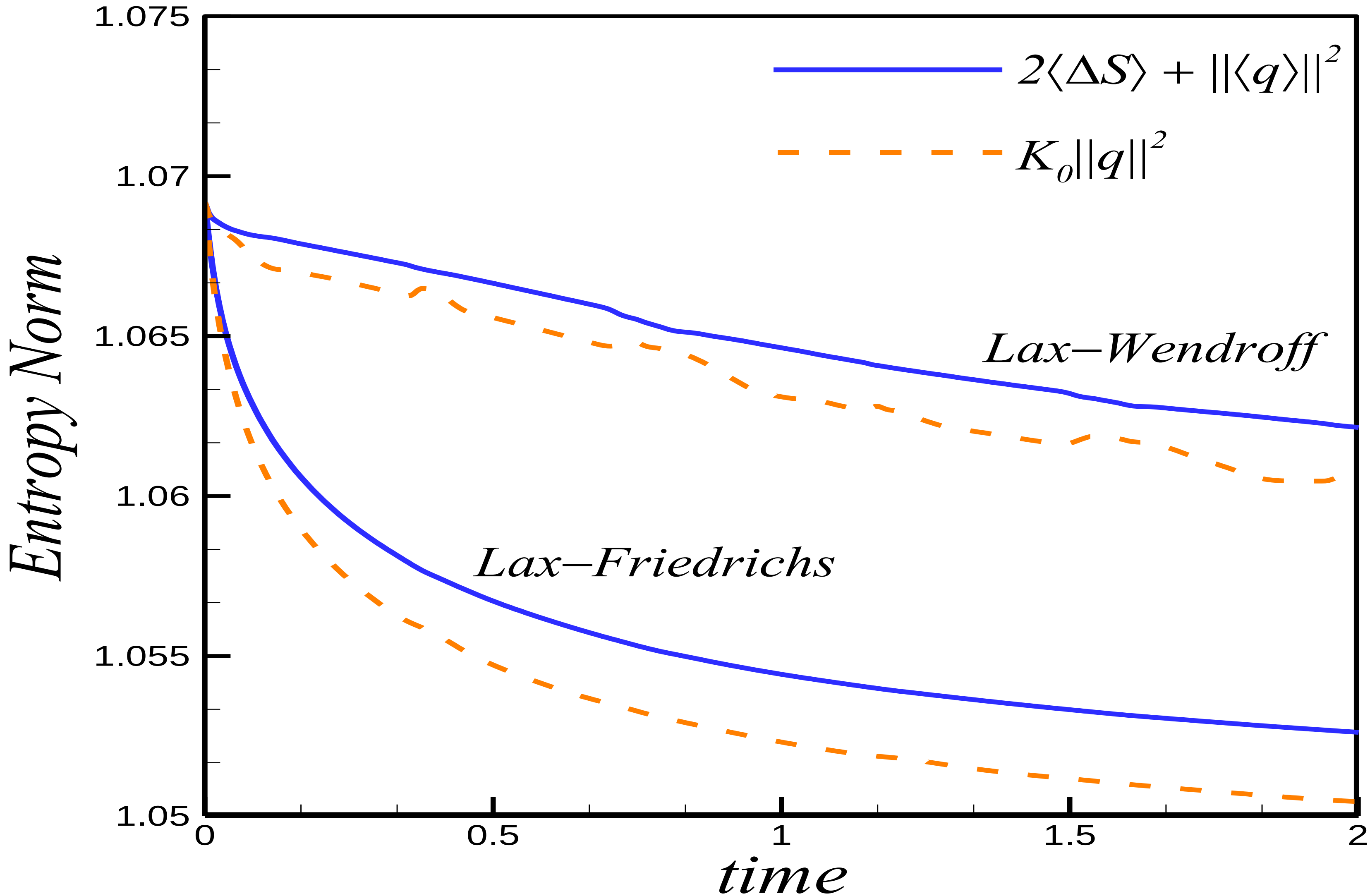
Linear Acoustic Perturbation



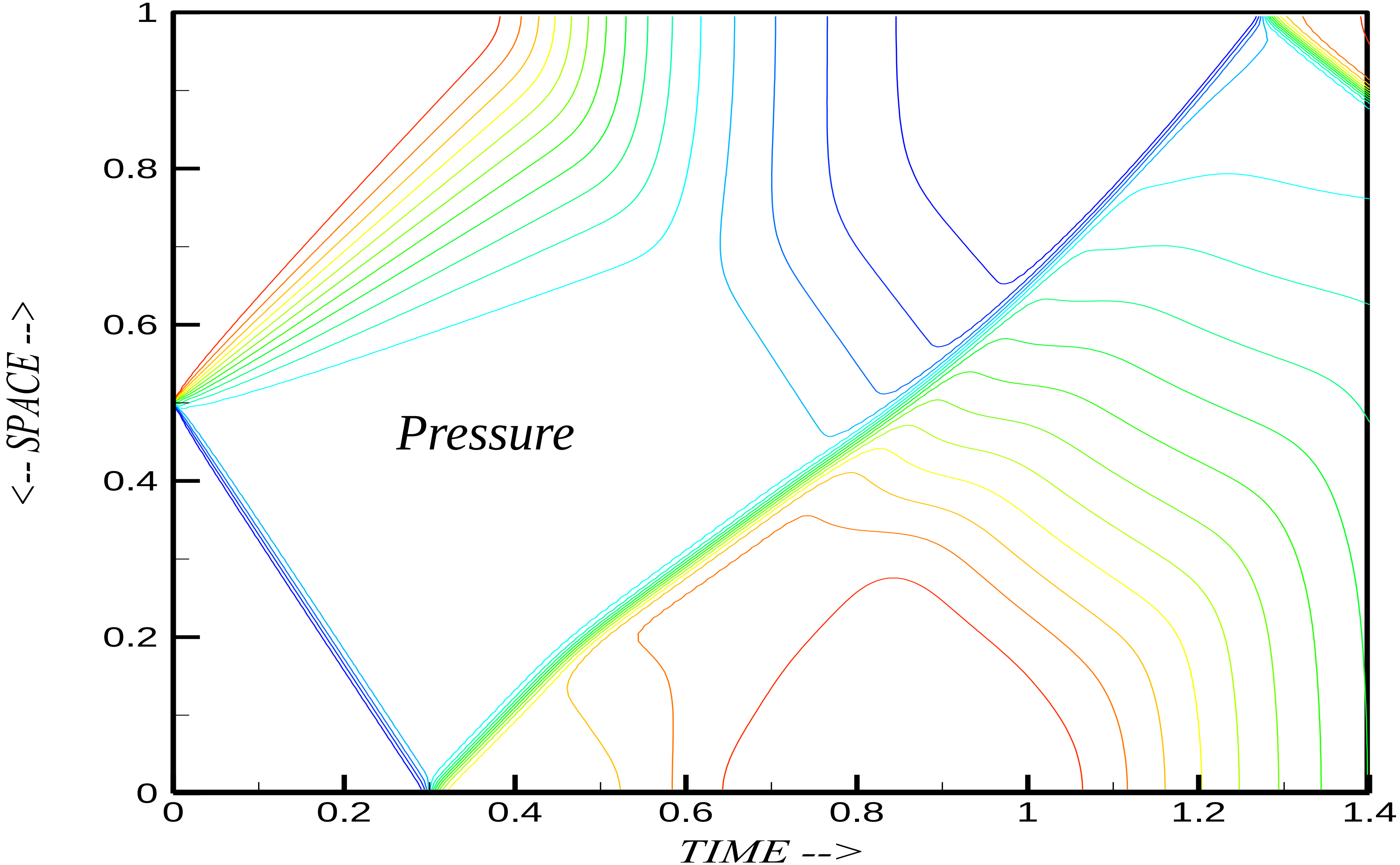
Entropy Generation for Acoustic Wave Simulation



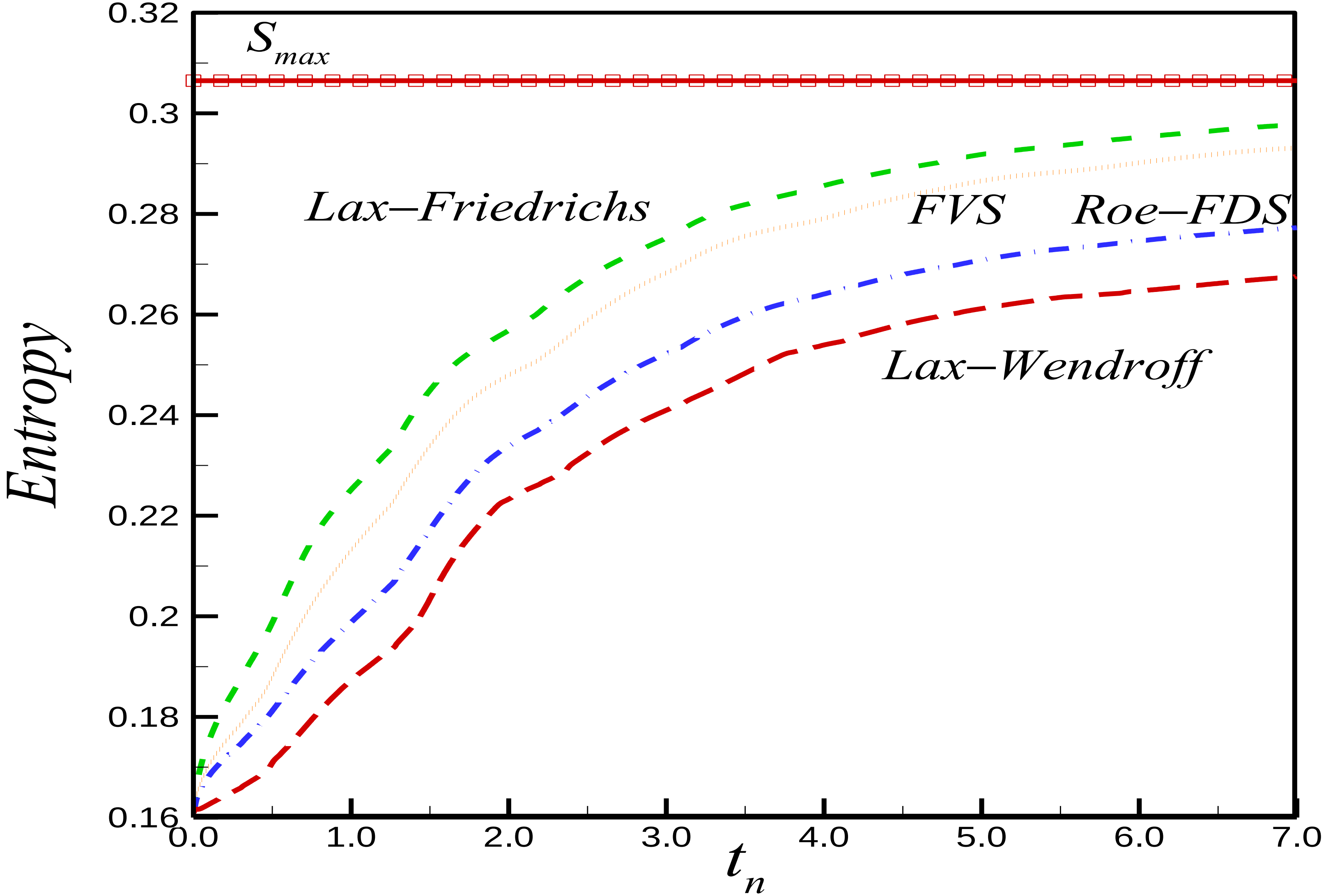
Numerical Stability as Measured by Metrics Established with SLT



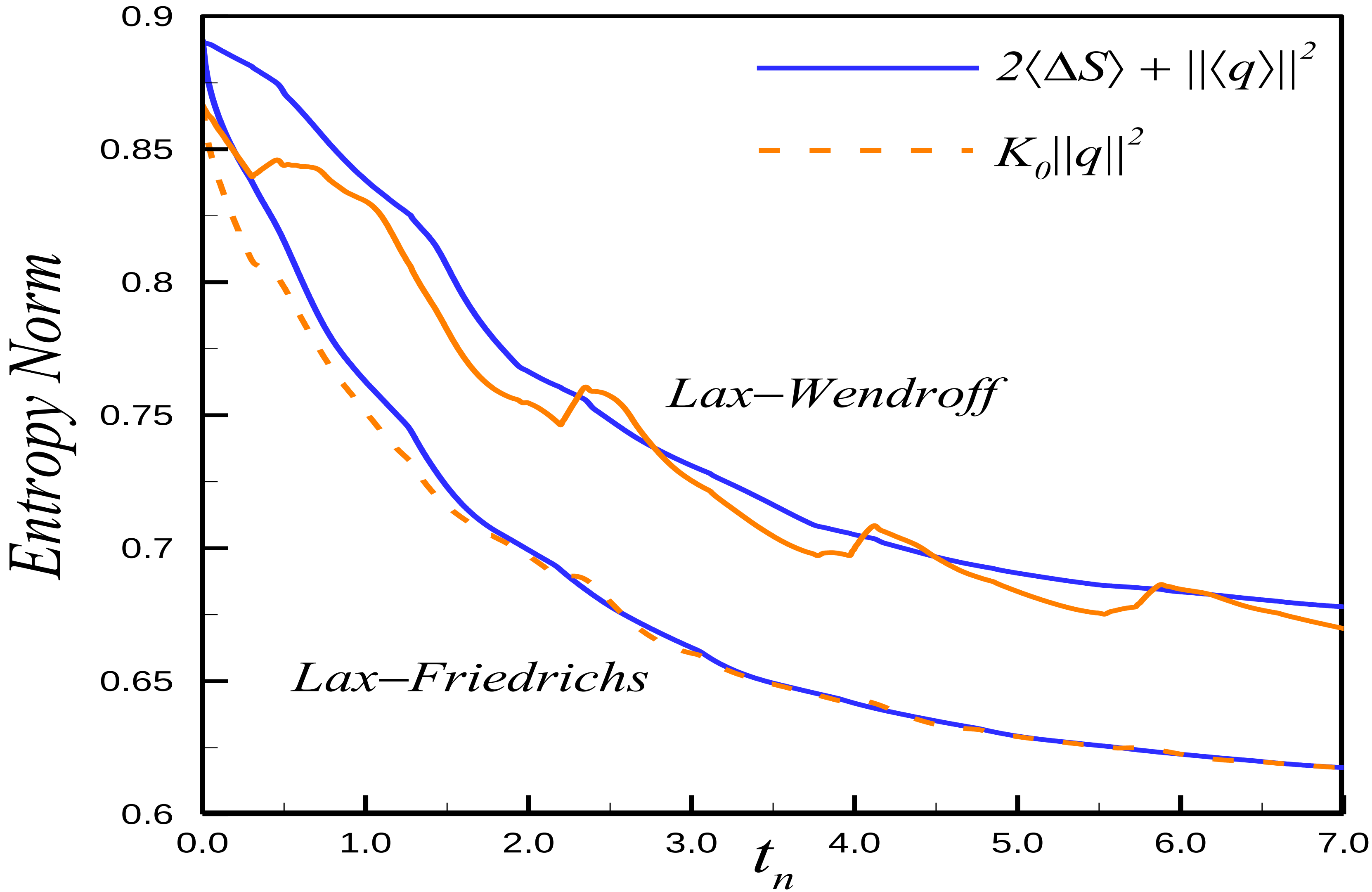
Nonlinear Shock Tube Simulation



Entropy Generation in Shock Tube



Numerical Stability as Measured by Metrics Established with SLT



General Entropy Principle

★ There exists a functional S such that

$$S_0 - S - \frac{\partial S}{\partial U}_0 \left(U_0 - U\right) - \frac{\partial S}{\partial V}_0 \left(V_0 - V\right) \geq 0$$

★ Thermodynamic definition of T and P:

$$\frac{1}{T} \equiv \frac{\partial S}{\partial U} \qquad \frac{P}{T} \equiv \frac{\partial S}{\partial V}$$

★ Concavity property quantifies exergy:

$$T_0\left(S_0 - S\right) - \left(U_0 - U\right) - P_0\left(V_0 - V\right) = X$$

Selected References

- Camberos, Jose A., “On the construction of entropy balance equations for arbitrary thermophysical processes,” *AIAA-2001-0815,* Reno, NV, Jan. 8-11, 2001
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- Camberos, Jose A., “Nonlinear time-step constraints based on the second law of thermodynamics,” *AIAA-1999-0558* Reno, NV, Jan. 11-14, 1999
- Camberos, J., “A Review of Numerical Methods in Light of the Second Law of Thermodynamics,” *AIAA-2007-405*, Miami, Florida, June 25-28, 2007

Inspiration

- **B. H. Lavenda, "Statistical Physics: A Probabilistic Approach"**
  - *Gauss' Error Law*
  - *Entropy Concavity ➔ Essence of 2nd Law*
- **E. T. Jaynes & MaxEnt**
  - *Construction of entropy function*
- **A. Bejan, "Entropy Generation Minimization"**

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The Second Law

CLOSING REMARKS

Conclusion & Implications

- ***True system-level analysis MUST use combined 1st & 2nd Laws!!***
- **Implications:**
  - *Analysis:*
    - Ensure analyses produce physically possible results
  - *Design:*
    - Provides guidance for more efficient optimizations
  - *Numerical Methods & 2nd Law*
    - Time-step restrictions for explicit methods
    - Numerical Stability
    - Convergence criteria