Theoretical Numerical Analysis

Scott Kruger

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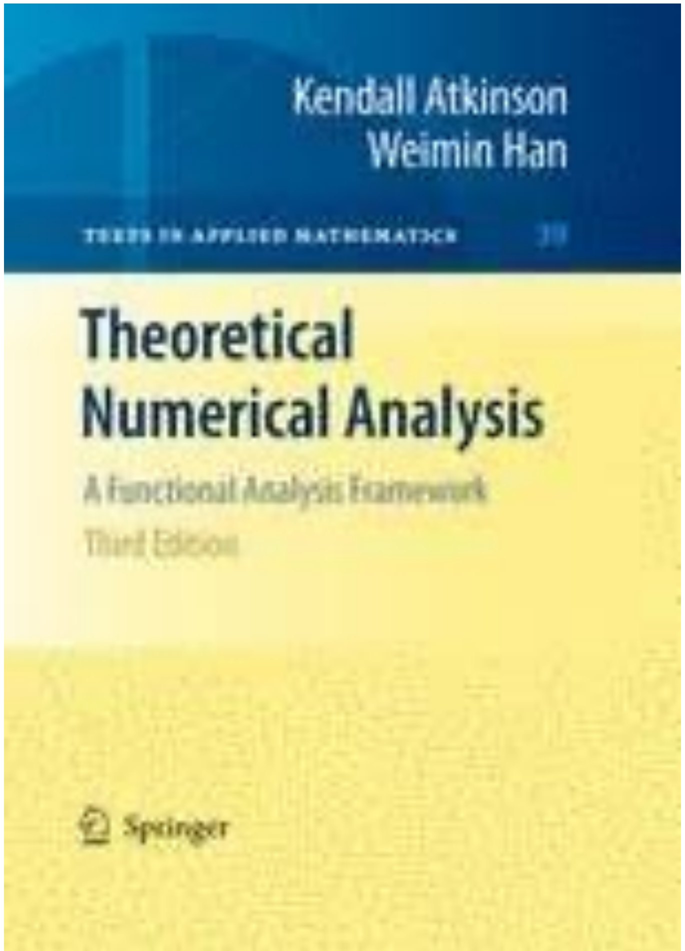
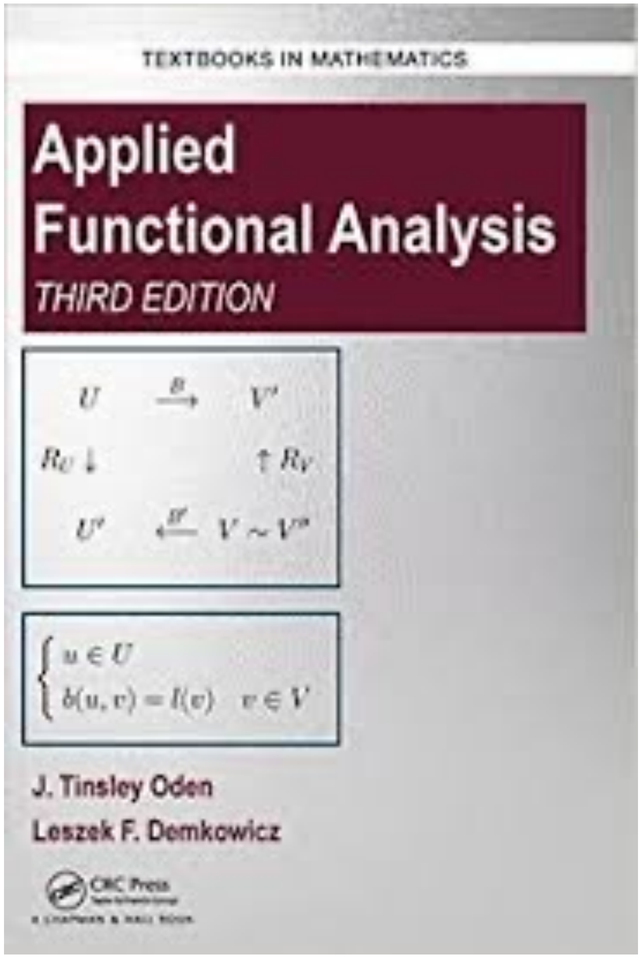
With many thanks to Eric Howell and Jake King

Or, stuff I wish I would have learned in grad school about numerical analysis

Good books on the topic





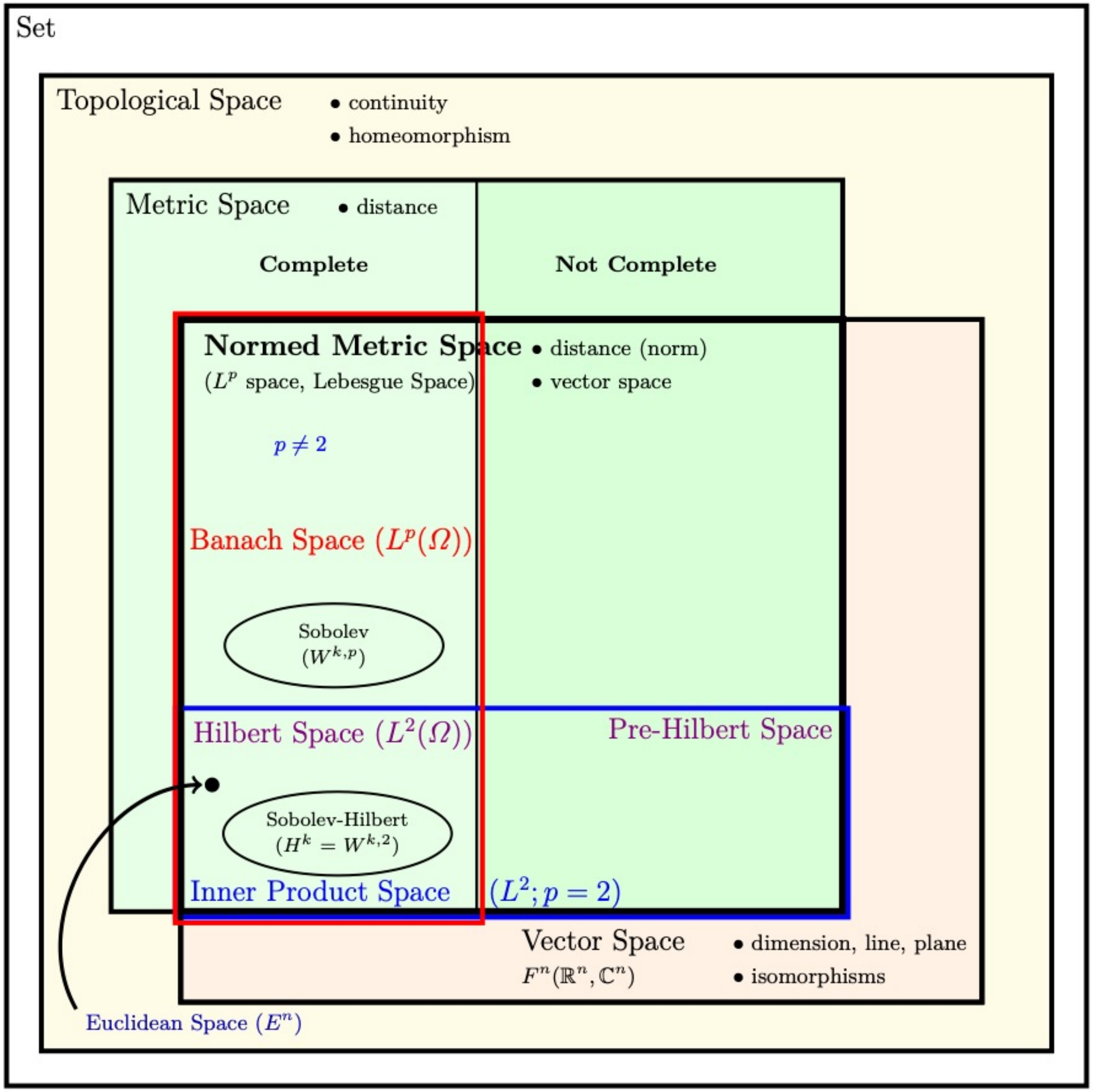
Outline

- Review of functional analysis
- Fundamental theorem of numerical analysis
- Weighted-residual methods (variational methods)
- Taxonomy of methods

Review of functional analysis

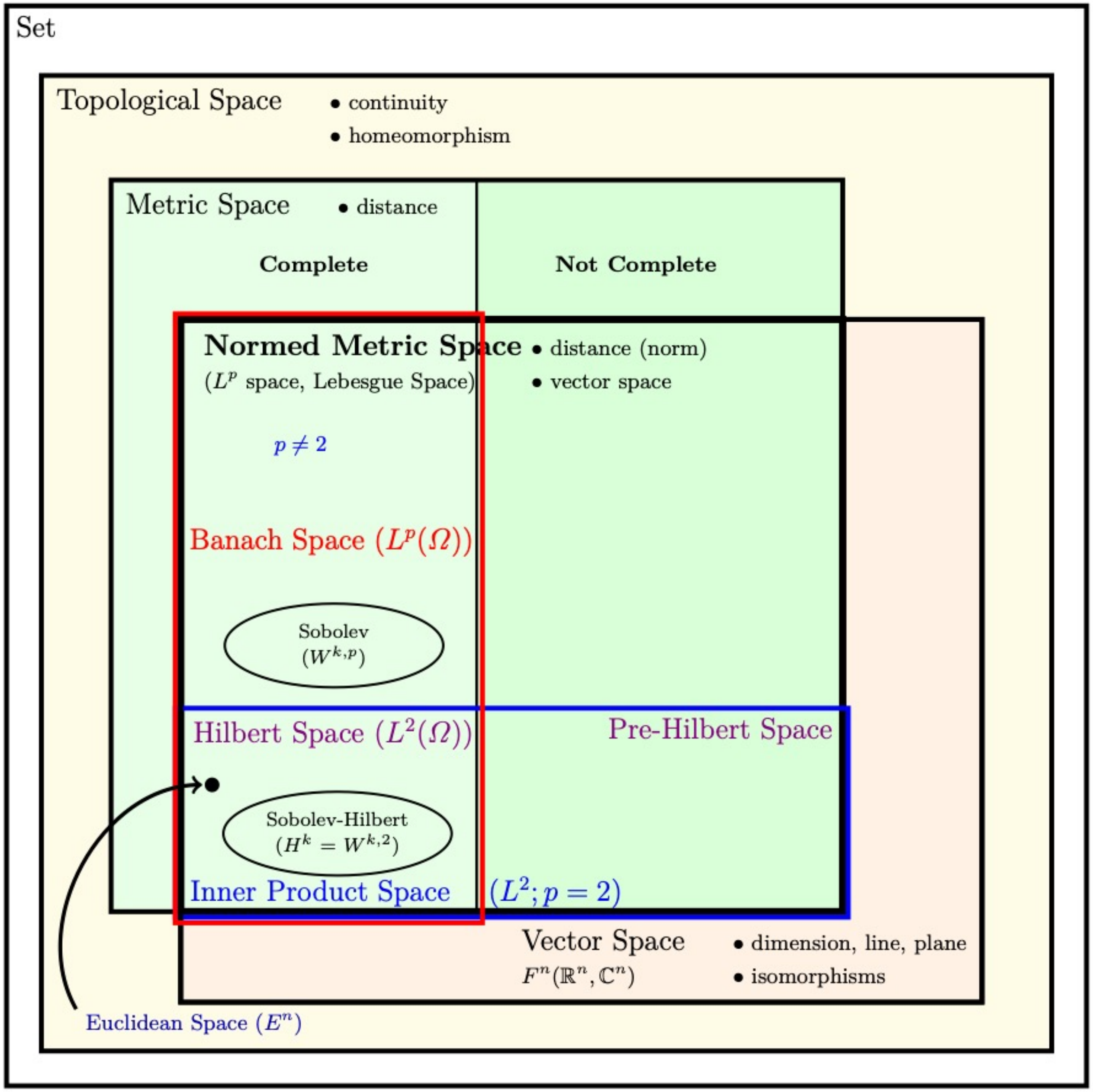
- Key idea:
  - Start with Euclidean space
  - Generalize to functions
  - Abstract and figure out the minimal thing required
  - Call that a new space
  - Keep abstracting

Functional spaces overview



- What you need to know:
  - Studying PDEs: Sobolev spaces
  - Sobolev space is a subset of Banach space
  - Most theorems of interest are in Banach space (because we need norms and distance)
  - Physics: Need inner products so generally in Hilbert space (think quantum mechanics)

Sobolev space



- Key to Sobolev space: the weak derivative

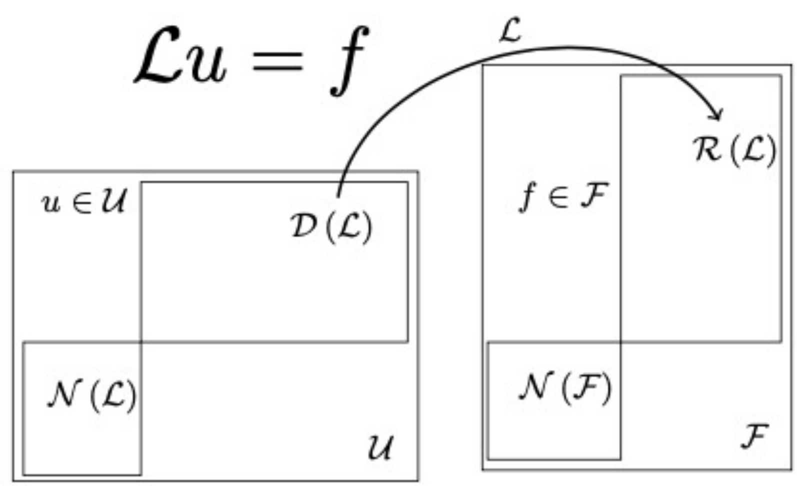
$$\int_\Omega u\, D^\alpha \varphi\, dx = (-1)^{|\alpha|} \int_\Omega \varphi\, D^\alpha u\, dx,$$

- Where: $$D^\alpha f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}}.$$

- It's what allows finite elements to fit into functional analysis
- Expands C^α space of traditional analysis
- Example: Laplace function requires C^2 in traditional analysis but C^1 finite elements OK because in Sobolev space

Generalized Numerical Analysis

- Consider general form for linear equations: $$\mathcal{L}u = f$$
- Use this for analysis (nonlinear and time-dependent equations can be fit into framework but can be more complicated)
- What spaces are of importance?



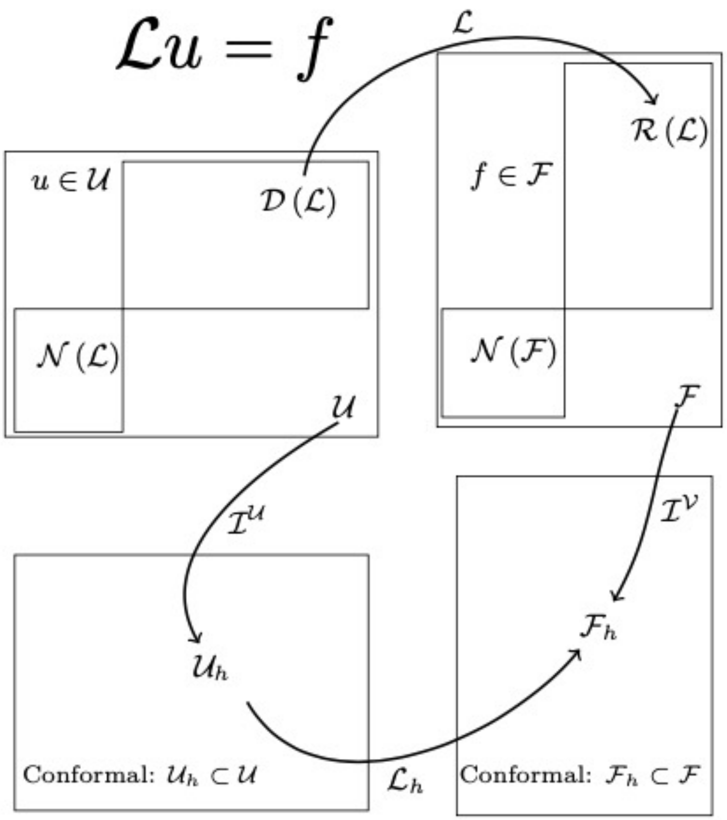
Continuous $(\mathcal{U})$**:**	Solution	**Continuous** $(\mathcal{F})$**:**	Data
Continuous $(\mathcal{D}(\mathcal{L}))$**:**	Domain	**Continuous** $(\mathcal{R}(\mathcal{L}))$**:**	Range or Image

Generalized Numerical Analysis: Issues with all numerical analysis schemes

- Steps to discretize equations:
  - Specify equations: $\mathcal{L}u = f$
  - Discretize equations: $\mathcal{L}_h u_h = f_h$
  - Solve equations: $u_h = {\mathcal{L}_h}^{-1} f_h$
- Want: $\text{Convergence } \|u_h - u\| \to 0$
- Hard to prove directly though.
- Fundamental theorem of numerical analysis (a.k.a, Lax equivalence theorem): *a discretization scheme that is consistent and stable is convergent.*

CONSISTENCY + STABILITY = CONVERGENCE

Discretization in terms of spaces



Continuous ($\mathcal{U}$):	Solution	**Continuous** ($\mathcal{F}$):	Data
Continuous ($\mathcal{D}(\mathcal{L})$):	Domain	**Continuous** ($\mathcal{R}(\mathcal{L})$):	Range or Image
Discrete ($\mathcal{U}_h$):	Discrete Solution	**Discrete** ($\mathcal{F}_h$):	Discrete Data
Matrix (A):	Row	**Matrix** (A^H):	Column

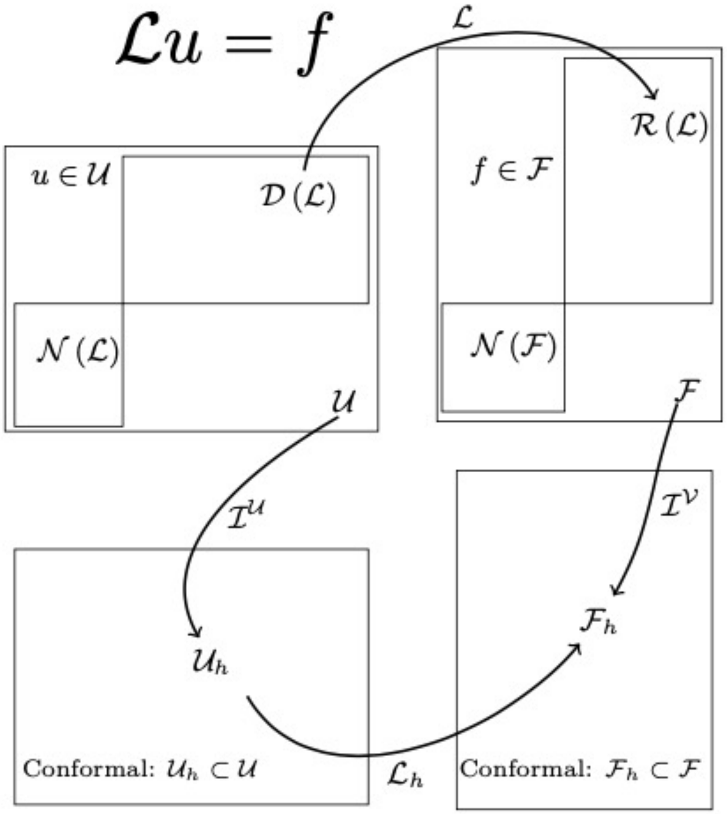
Consistency

Discretize equation: $\mathcal{L}_h u_h = f_h$

$$\|\mathcal{L}_h u_h - f_h\| = \left\|\mathcal{L}_h \mathcal{I}^{\mathcal{U}} u - \mathcal{I}^{\mathcal{V}} \mathcal{L} u\right\| \leq C_h^{cons} h^r;$$

Discretization in terms of spaces

$$\mathcal{L}u = f$$



Consistency

Discretize equation: $\mathcal{L}_h u_h = f_h$

$$\|\mathcal{L}_h u_h - f_h\| = \left\|\mathcal{L}_h \mathcal{I}^{\mathcal{U}} u - \mathcal{I}^{\mathcal{V}} \mathcal{L} u\right\| \leq C_h^{cons} h^r,$$

Stability

Solve equation: $u_h = \mathcal{L}_h{}^{-1} f_h$

$$\frac{\text{solution perturbation}}{\text{data perturbation}} = \frac{\|\tilde{u_h} - u_h\|_h}{\left\|\tilde{f}_h - f_h\right\|_h} = \frac{\left\|\mathcal{L}_h{}^{-1}\epsilon_h\right\|_h}{\|\epsilon_h\|_h}$$

$$C_h^{stab} = \sup_{0 \neq \epsilon_h in \mathcal{F}_h} \frac{\left\|\mathcal{L}_h{}^{-1}\epsilon_h\right\|_h}{\|\epsilon_h\|_h} = \left\|\mathcal{L}_h{}^{-1}\right\|_{\mathcal{L}(\mathcal{U}_h, \mathcal{F}_h)}$$

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Proof of generalized Lax equivalence theorem

- Proof of equivalence theorem:

$$u - u_h = \mathcal{L}_h{}^{-1}\left[\mathcal{L}_h(u-u_h)\right] = \mathcal{L}_h{}^{-1}\left[\mathcal{L}_h u - \mathcal{L}_h u_h\right] = \mathcal{L}_h{}^{-1}\left[\mathcal{L}_h u - f_h\right]$$

- Taking norm:

$$\begin{aligned}\|u - u_h\| &= \left\|\mathcal{L}_h{}^{-1}\right\| \left[\left\|\mathcal{L}_h \mathcal{I}^{\mathcal{U}} u - \mathcal{I}^{\mathcal{V}} \mathcal{L} u\right\|\right] \\ &\leq C_h^{stab} C_h^{cons} h^r,\end{aligned}$$

- These constants have continuous equivalents and one can define a condition number in terms of them:

$$\kappa(\mathcal{L}) = C^{stab} C^{cons}$$

  - That is, hard problems are hard regardless of discretization scheme

Weighted-residual methods or variational methods

- Finite elements, spectral methods, polynomial methods, … are all types of weighted-residual methods

$$(\mathcal{L}u, v) = (f, v)$$

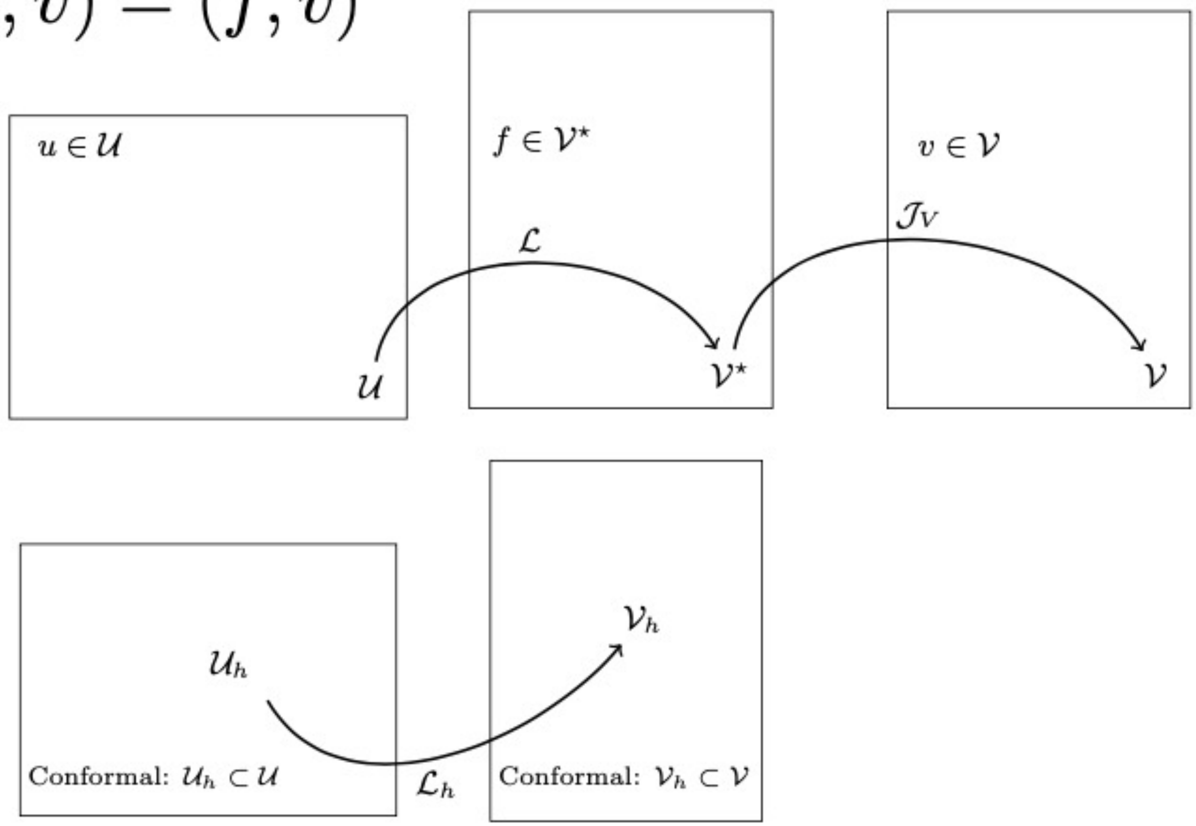
- These are all projection methods: Project trial space onto test space
- These are also written in terms of bilinear forms:

$$B(u, v) = F \qquad\qquad B(:,:) : \mathcal{U} \times \mathcal{V} \to \mathbb{R}$$

where $B(u, v) = (\mathcal{L}u, v)$.

Spaces view of weighted-residual methods

$$B(u, v) = (f, v)$$



Continuous ($\mathcal{U}$): Solution
Discrete ($\mathcal{U}_h$): Trial
Matrix (A): Row

Continuous ($\mathcal{V}^\star$): Data
Discrete ($\mathcal{V}_h$): Test
Matrix (A^H): Column

Lax equivalence theorem for WRM given by Lax-Milgram theorem

- A bilinear form is *continuous* if it satisfies :

$$B\left(u,u\right) \leq C^{conty}\left\|u\right\|\left\|v\right\|$$

- And *coercive* (or V-elliptic) if it satisfies :

$$C^{coerce}\left\|u\right\|^{2} \leq B\left(u,u\right)$$

- Lax-Milgram: *if a bilinear operator is continuous and coercive, then there is a unique solution to the variational problem, B(u,v)=F, and a unique solution to the discrete equivalents.*
- In terms of previous discussion:
  - Continuity constant is the consistency constant
  - Coercive constant is the stability constant
- All we need are continuous and coercive methods

Approaches to coercivity

- Symmetric problems work well because they can be cast as finding the minimum of a quadratic energy functional (truly a variational problem)
- Non-symmetric problems: become saddle point problems (more difficult to find correct stationary point)
- Also consider this problem:

$$\frac{\partial u}{\partial t} + \nabla \cdot \boldsymbol{F}(u) = S$$

can show that if $\boldsymbol{F}''(u) > 0$
then discontinuities arise

  - Are your discrete spaces large enough capture these discontinuities?

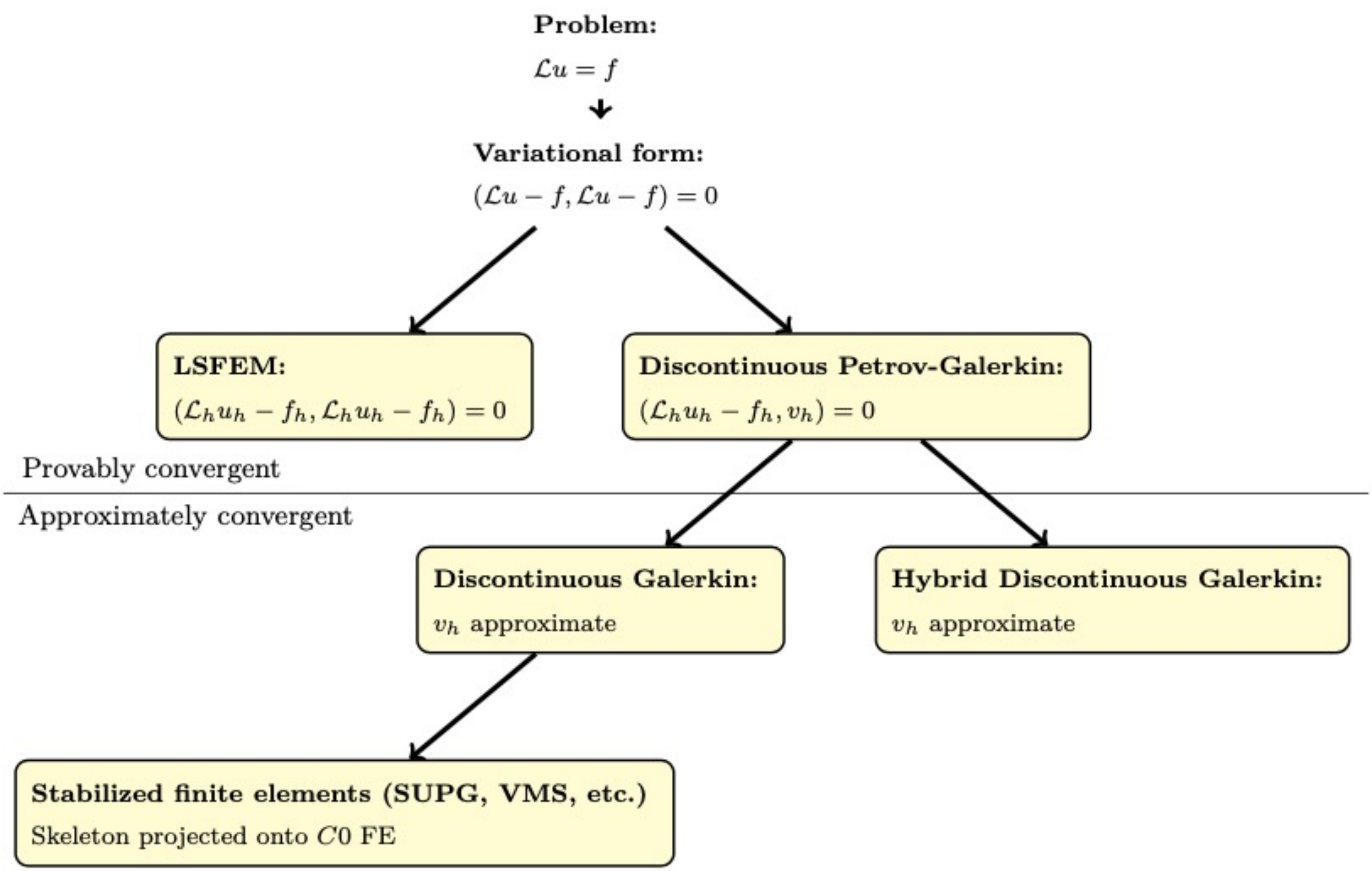
Two related approaches have emerged to handle non-symmetric systems

- Least-squares: $$E(u; f) = (\mathcal{L}u - f, \mathcal{L}u - f)$$
  - Solves saddle point problem.
    - However, typically done with continuous (C^0 elements)
  - Discrete Least Squares (DLS):
    Enable discontinuous test functions (relatively immature)
- Discontinuous Petrov-Galerkin (DPG)

$$(\mathcal{L}u_h - f_h, v_h) = 0,$$

  - Calculate v_h such that coercivity is guaranteed
    - Theoretically perfect! However, in practice:
      - Calculations are really global, but approximations are made to make it local to save computational time
      - Should be updated every time step – again, too computationally expensive

Hierarchy of approximations



Summary

- Atkinson and Han is a good book if you are interested in these topics
  - Approach and figures presented here actually not in book but based on other references (Arnold, Kirby)
- For 99% of what you do, you only have to worry about Sobolev-Hilbert space, but most literature operates in Banach space to be most general. You can use Banach space proofs.
- No perfect scheme exists and the “best” ones are often too expensive to be practical

Some key authors influencing this talk

- Demkowiscz (Oden Institute)
  - Discontinuous Petrov-Galerkin, theoretical numerical analysis
- Tan Bui-Thanh (Oden Institute)
  - DPG, Hybridized DG, …
- Paul Bochev (Sandia NL)
  - Mimetic discretization, stabilized FE, LSFEM
- D. Arnold (U. Minnesota)
  - Mimetic finite elements, DG, theoretical numerical analysis
- TJR Hughes (Oden Institute)
  - Streamline-Upwind Petrov Galerkin (SUPG), VMS
- Robert Kirby (Baylor)
  - Mimetic finite elements, theoretical numerical analysis