Structure-preserving discretizations for the radiative transfer equation

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1. Radiative transfer

We consider the **scalar radiative transfer equation** (RTE):

$$\begin{cases} \frac{\partial \rho}{\partial t} + [H,\rho] + \Sigma(\mathbf{x},|\mathbf{k}|)\rho = \int_{|\mathbf{k}'|=|\mathbf{k}|} \sigma(\mathbf{x},\mathbf{k}'\cdot\mathbf{k})\rho(\mathbf{x},\mathbf{k}',t)d\mathbf{k}', & \text{in } \Omega \\ \rho(\mathbf{x},\mathbf{k},0) = \rho_0(\mathbf{x},\mathbf{k}), \end{cases}$$

with

$$[f,g] = \nabla_{\mathbf{k}} f \cdot \nabla_{\mathbf{x}} g - \nabla_{\mathbf{x}} f \cdot \nabla_{\mathbf{k}} g, \qquad H = v(\mathbf{x})|\mathbf{k}|, \qquad \Omega = \mathbb{R}^3 \times \mathbb{R}^3 \backslash \{0\}.$$

This equation models the propagation of light through a material with a varying refractive index indicated by the local velocity $v(\mathbf{x})$, taking into account the processes of refraction and scattering.

It has applications in several fields such as medical imaging[1] and atmospherical science[2].

2. Metriplectic formulation

Many PDEs describing physical processes satisfy:

1. Conservation of energy,
2. Dissipation of entropy.

Metriplectic formulation[3]**:** Reformulate equations into a bracket equation for functionals:

$$\frac{\partial \rho}{\partial t} = A\rho \quad \to \quad \frac{\partial F[\rho]}{\partial t} = \{F,G\} + (F,G),$$

where A is a (nonlinear) operator,

$\{\cdot,\cdot\}$ is the **Symplectic** bracket. It is bilinear, anti-symmetric and satisfies the Jacobi identity,

$(\cdot,\cdot)$ is the **Metric** bracket. It is bilinear, symmetric and negative semidefinite,

G is the free energy functional $G = H + S$,

H is the **energy** functional, a Casimir of $(\cdot,\cdot)$, i.e.: $(H,A) = 0 \quad \forall A$,

S is the **entropy** functional, a Casimir of $\{\cdot,\cdot\}$, i.e.: $\{S,A\} = 0 \quad \forall A$,

Then it follows that

$$\frac{\partial H}{\partial t} = 0, \qquad \frac{\partial S}{\partial t} \leq 0.$$

3. Metriplectic formalism for the RTE

The RTE can be reformulated into the metriplectic formulation as[4]

$$\frac{\partial}{\partial t} F_\eta[\rho] = \Big\{F_\eta, G\Big\} + \Big(F_\eta, G\Big),$$

with

$$\Big\{A,B\Big\} = \int_\Omega \rho \left[\frac{\delta A}{\delta \rho}, \frac{\delta B}{\delta \rho}\right] d\Omega,$$

$$\Big(A,B\Big) = \frac{1}{4}\int_\Omega \int_{\mu'} r^2 \sigma(z) \left(\frac{\delta A}{\delta \rho'} - \frac{\delta A}{\delta \rho}\right) \cdot \left(\frac{\delta B}{\delta \rho} - \frac{\delta B}{\delta \rho'}\right) d\mu' d\Omega,$$

$$F_\eta = \int_\Omega \eta\rho d\Omega, \qquad G = H + S,$$

$$H = \int_\Omega \rho v(\mathbf{x})|\mathbf{k}| d\Omega, \qquad S = \int_\Omega \rho^2 d\Omega.$$

4. Discretization

For numerical purposes we consider the RTE in a slab geometry with isotropic scattering:

$$\frac{\partial \rho}{\partial t} + [H,\rho] + r^2\sigma(z)\rho = r^2 \frac{\sigma(z)}{2} \int_{-1}^{1} \rho(z,r,\mu',t)d\mu'.$$

$$z \in (-\infty,\infty), \quad r = |\mathbf{k}| \in (0,\infty), \quad \mu = \frac{k_z}{|\mathbf{k}|} \in [-1,1],$$

$$[H,\rho] = v(z)\mu\frac{\partial \rho}{\partial z} - \frac{\partial v}{\partial z}\mu r \frac{\partial \rho}{\partial r} - \frac{\partial v}{\partial z}(1-\mu^2)\frac{\partial \rho}{\partial \mu}.$$

Discretization:

- Discretize $\rho \to \rho_h = \sum_{i=1}^N \hat{\rho}_i \varphi_i(z,r,\mu) = \hat{\rho}^T \varphi$,
- Functionals: $F[\rho_h] = \hat{F}(\hat{\rho}) \to \frac{\delta F[\rho_h]}{\delta \rho} = \frac{\partial \hat{F}}{\partial \hat{\rho}} \mathbb{M}^{-1}\varphi = \nabla \hat{F}^T \varphi$,
- Discrete brackets become

$$\Big\{\hat{A},\hat{B}\Big\}_h = \nabla \hat{A}^T \mathbb{P}(\hat{\rho}) \nabla \hat{B},$$
$$\Big(\hat{A},\hat{B}\Big)_h = \nabla \hat{A}^T \mathbb{S} \nabla \hat{B}.$$

with

$$\mathbb{P}_{i,j}(\hat{\rho}) = \int_\Omega \rho_h \left[\varphi_i, \varphi_j\right] d\Omega,$$

$$\mathbb{S}_{i,j} = \frac{1}{4}\int_\Omega \int_{\mu'} r^2 \sigma(z) \left(\varphi_i(\mu') - \varphi_i(\mu)\right)\left(\varphi_j(\mu) - \varphi_j(\mu')\right) d\mu' d\Omega.$$

5. Results

Discrete Hamiltonian:

$$\hat{H}(\hat{\rho}) = \sum_{i=1}^N \int_\Omega v(z) r \varphi_i d\Omega.$$

if $v(z)r$ is in the approximation space, i.e. $v(z)r = \sum_{i=1}^n \hat{h}_i \varphi_i$ then

$$\hat{H} = \hat{h}^T \mathbb{M} \hat{\rho},$$

Energy conservation and entropy dissipation follow on the semi-discrete level by plugging this expression into the brackets and noting that

$$\mathbb{P}\hat{\rho} = \mathbb{S}\hat{h} = 0.$$

The discrete equation for $\hat{\rho}$ can be written as

$$\mathbb{M}\frac{\partial \hat{\rho}}{\partial t} = \mathbb{H}\hat{\rho} + \mathbb{S}\hat{\rho}, \quad \mathbb{H} = \int_\Omega \varphi_j \left[v(z)r, \varphi_i\right] d\Omega$$

On a fully discrete level structure-preservation is obtained by the **midpoint rule**:

$$\mathbb{M}\frac{\hat{\rho}_{n+1} - \hat{\rho}_n}{\Delta_t} = \frac{1}{2}(\mathbb{H} + \mathbb{S})(\hat{\rho}_n + \hat{\rho}_{n+1}).$$

6. Further work

- Extend metriplectic formulation to radiative transfer with polarization.
- Incorporate boundary conditions into the formalism.

7. References

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