Nonintrusive Manufactured Solutions for Non-Decomposing Ablation in Two Dimensions

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Outline

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- Introduction
  - Ablation
  - Verification and Validation
  - Code Verification
  - Nonintrusive Manufactured Solutions
- Governing Equations
- Manufactured Solutions
- Heat Equation Solution
- Boundary Condition Reconciliation
- Numerical Examples
- Summary

Ablation

Ablative processes are important in many scientific and engineering problems

- Glacial erosion, fire protection, medical procedures, and industrial manufacturing processes
- Ablative materials used as sacrificial heat shields for weapons, rockets, and hypersonic reentry vehicles
  - Accurate prediction of mass and energy loss necessary to minimize weight and cost of heat shield
  - Changes in outer mold line from surface erosion important in hypersonic flight
- Establishing credibility in ablative models is essential

Verification and Validation

Credibility of computational physics codes requires verification and validation

- **Validation** assesses how well models represent physical phenomena
  - Computational results are compared with experimental results
  - Assess suitability of models, model error, and bounds of validity

- **Verification** assesses accuracy of numerical solutions against expectations
  - *Solution verification* estimates numerical error for particular solution
  - *Code verification* verifies correctness of numerical-method implementation

Code Verification

Code verification is focus of this work

- Governing equations are numerically discretized
  - Discretization error is introduced in solution
- Seek to verify discretization error decreases with refinement of discretization
  - Should decrease at an expected rate
- Use manufactured and/or exact solutions to compute error

Code Verification

Code verification demonstrated in many computational physics disciplines

- Fluid dynamics
- Solid mechanics
- Heat transfer
- Multiphase flows
- Electrodynamics
- Electromagnetism
- Fluid–structure interaction
- Radiation hydrodynamics

Existing ablation code verification has used simple exact solutions

We present an approach for developing nonintrusive manufactured solutions

- Manufactured solutions more thoroughly test code capabilities
- Approach does not require code modification
- Instead of introducing a source term, we manufacture ablation parameters

Nonintrusive Manufactured Solutions

- Optionally transform governing equations
- Derive solutions that satisfy nonablating boundary conditions
- Manufacture parameters to satisfy ablating boundary condition

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  - Heat Conduction
  - Ablation and Boundary Conditions
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Heat Conduction

For a solid, the energy equation due to heat conduction is

$$\frac{\partial}{\partial t}(\rho e) + \nabla \cdot \mathbf{q} = 0$$

Internal energy e and heat flux $\mathbf{q}$ are modeled by

$$e = e_0 + \int_{T_0}^{T} c_p(\hat{T})d\hat{T}, \qquad \mathbf{q} = -k(T)\nabla T$$

The heat equation is

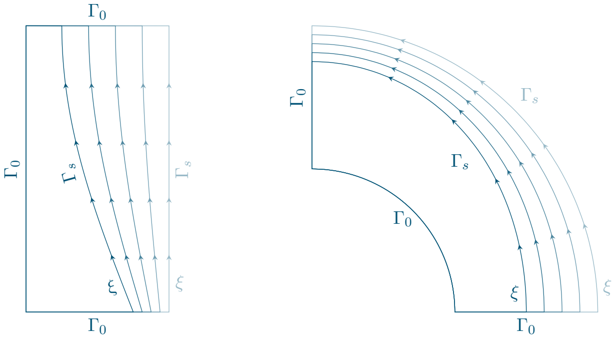
$$\rho c_p(T)\frac{\partial T}{\partial t} - \nabla \cdot (k(T)\nabla T) = 0$$

ρ is constant density
$c_p(T)$ is specific heat capacity
$k(T)$ is thermal conductivity of isotropic material

Ablating Surface Parameterization

Time-dependent material domain is $\Omega(t)$ with boundary $\Gamma = \Gamma_s \cup \Gamma_0$

- Γ_s is ablating surface: $\Gamma_s = \{(x, y) : x = x_s,\ y = y_s\}$
  - arbitrarily parameterized by $\mathbf{x}_s(\xi, t) = (x_s(\xi, t), y_s(\xi, t))$
  - $\xi \in [0, 1]$ increases in counterclockwise direction
- Γ_0 is non-ablating surface



Recession Definition

Along Γ_s, material recedes by $s(\xi, t)$ in direction opposite to outer normal

Recession rate defined by

$$\dot{s}(\xi, t) = -\frac{\partial \mathbf{x}_s}{\partial t}(\xi, t) \cdot \mathbf{n}_s(\xi, t),$$

where the outer unit normal vector is defined by

$$\mathbf{n}_s(\xi, t) = \frac{1}{\sqrt{(\partial x_s/\partial \xi)^2 + (\partial y_s/\partial \xi)^2}} \frac{\partial}{\partial \xi} \begin{Bmatrix} y_s \\ -x_s \end{Bmatrix}$$

Recession Rate and Heat Flux Modeling

Recession rate modeled by $\dot{s}(\xi, t) = \dfrac{B'(T_s, p_e)C_e}{\rho}$

Heat flux along ablating surface $q_s = \mathbf{q}_s \cdot \mathbf{n}_s$ modeled by

$$q_s = \underbrace{C_e\left[h_w(T_s, p_e) - h_r\right]}_{\text{convective heat flux}} + \underbrace{\rho\dot{s}\left[h_w(T_s, p_e) - h_s(T_s)\right]}_{\text{energy loss from ablation}} + \underbrace{\epsilon\sigma\left(T_s^4 - T_r^4\right)}_{\text{radiative flux}}$$

$T_s(\xi, t) = T(\mathbf{x}_s(\xi, t), t)$ is temperature along ablating surface
$p_e(\xi, t)$ is pressure at outer edge of boundary layer
$B'(T_s, p_e)$ is nondimensionalized char ablation rate
$C_e(\xi, t)$ is heat transfer coefficient $(\rho_e u_e C_h)$
$h_w(T_s, p_e)$ is wall enthalpy
$h_r(\xi, t)$ is recovery enthalpy
$h_s(\xi, t)$ is solid enthalpy, computed from $h_s(T_s) = h_0 + \int_{T_0}^{T_s} c_p(\hat{T})d\hat{T}$
ϵ is emissivity
σ is Stefan–Boltzmann constant
$T_r = 300$ K is radiation reference temperature

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  - Discretization Error
  - Solutions
  - Manufactured Solutions from Manufactured Parameters
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Discretization Error

A governing system of equations can be written generally as

$$\mathbf{r}(\mathbf{u};\boldsymbol{\mu}) = \mathbf{0}$$

$\mathbf{r}$ represents equations, $\mathbf{u}(\mathbf{x},t)$ is state vector, and $\boldsymbol{\mu}$ is parameter vector

Discretize in time and space to get

$$\mathbf{r}_h(\mathbf{u}_h;\boldsymbol{\mu}) = \mathbf{0}$$

$\mathbf{r}_h$ is residual of discretized equations and $\mathbf{u}_h$ is solution to discretized equations

Discretization error is $\mathbf{e}_\mathbf{u} = \mathbf{u}_h - \mathbf{u}$, and its norm $\|\mathbf{e}_\mathbf{u}\| \approx Ch^p$

C is function of solution derivatives
h is measure of discretization size
p is order of accuracy

Convergence studies of $\|\mathbf{e}_\mathbf{u}\|$ to measure p

Solutions

$\mathbf{e}_{\mathbf{u}}$ can only be measured if $\mathbf{u}$ is known

Exact solutions

- Negligible implementation effort: $\mathbf{r}(\mathbf{u}_{\text{Exact}}; \boldsymbol{\mu}) = \mathbf{0}$
- Limited cases, span small subset of application space

Manufactured solutions from forcing vector

- Do not satisfy original equations: $\mathbf{r}(\mathbf{u}_{\text{MS}}; \boldsymbol{\mu}) \neq \mathbf{0}$
- Require source term: $\mathbf{r}_h(\mathbf{u}_h; \boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}_{\text{MS}}; \boldsymbol{\mu})$
- Manufactured to exercise features of interest

Manufactured solutions from manufactured parameters

- Favorable properties similar to traditional manufactured solutions
- Negligible implementation effort: $\mathbf{r}(\mathbf{u}; \boldsymbol{\mu}_{\text{MP}}) = \mathbf{0}$

Manufactured Solutions from Manufactured Parameters

- Manufactured parameters do not require code modification
- Compute $\mathbf{u}$ from solutions to governing equations
- For unsatisfied boundary conditions, manufacture underlying parameters

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  - Time Dependency
  - Cartesian Coordinates
  - Polar Coordinates
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Heat Equation Solution

For $k(T) = \bar{k} f(T)$ and $c_p(T) = \bar{c}_p f(T)$, heat equation is

$$\frac{\partial \theta}{\partial t} - \bar{\alpha} \Delta \theta = 0,$$

where $\theta = \int_T f(T') dT' + C_k = F(T)$ (Kirchhoff transformation)

Disregard time dependency of domain and assume we can separate variables:

$$\theta(\mathbf{x}, t) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \hat{\theta}_{i,j}(t) \varphi_{i,j}(\mathbf{x})$$

$\varphi_{i,j}(\mathbf{x})$ is orthogonal basis
i and j are indices associated with the basis of different spatial coordinates

Time Dependency

Inserting solution expression into equation yields

$$\frac{1}{\bar{\alpha}}\frac{\hat{\theta}'_{i,j}(t)}{\hat{\theta}_{i,j}(t)} = \frac{\Delta\varphi_{i,j}(\mathbf{x})}{\varphi_{i,j}(\mathbf{x})} = -\lambda_{i,j}$$

For the time dependency,

$$\hat{\theta}_{i,j}(t) = \hat{\theta}_{i,j_0} e^{-\bar{\alpha}\lambda_{i,j}t}$$

Interested in $\lambda_{i,j} < 0$

- Focusing on ablative processes and interested in verifying time integrator
- Interested in cases where temperature increases with time

Cartesian Coordinates

Separate x and y dependencies:

$$\varphi_{i,j}(\mathbf{x}) = u_i(x)v_j(y)$$

From $v_j'(0) = v_j'(H) = 0$,

$$v_j(y) = \cos(j\pi y/H)$$

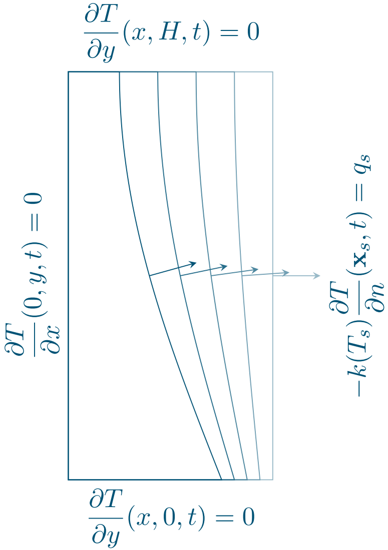
From $u'(0) = 0$,

$$u_i(x) = \begin{cases} \cosh(|\mu_i| x) & \text{for } \mu_i^2 < 0 \\ \cos(\ \mu_i\ x) & \text{for } \mu_i^2 \geq 0 \end{cases}$$

μ_i depends on BC at $x = x_s$, and

$$\lambda_{i,j} = \mu_i^2 + \nu_j^2,$$

where $\nu_j = j\pi/H$



Polar Coordinates

Partially separate r and ϕ dependencies:

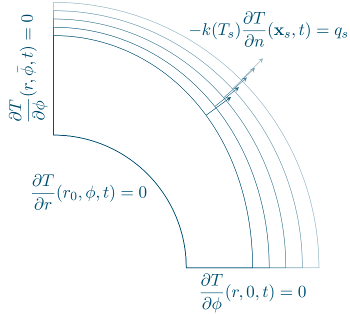
$$\varphi_{i,j}(\mathbf{x}) = u_{i,j}(r)v_j(\phi)$$

From $v_j'(0) = v_j'(\bar{\phi}) = 0$,

$$v_j(\phi) = \cos(j\pi\phi/\bar{\phi})$$

From $u'(r_0) = 0$ and letting $r' = \sqrt{|\lambda_{i,j}|}r$,

$$u_{i,j}(r) = \begin{cases} K_{i,j}I_{\nu_j}(r') + I_{i,j}K_{\nu_j}(r') & \text{for } \lambda_{i,j} < 0 \\ Y_{i,j}J_{\nu_j}(r') + J_{i,j}Y_{\nu_j}(r') & \text{for } \lambda_{i,j} > 0 \\ \cosh(\nu_j \ln(r/r_0)) & \text{for } \lambda_{i,j} = 0 \end{cases}$$



$\lambda_{i,j}$ depends on boundary condition at $r = r_s$, and $\nu_j = j\pi/\bar{\phi}$

I_α and K_α are modified Bessel functions of 1st and 2nd kind

$$K_{i,j} = K_{\nu_j-1}(r_0') + K_{\nu_j+1}(r_0')$$
$$I_{i,j} = I_{\nu_j-1}(r_0') + I_{\nu_j+1}(r_0')$$

J_α and Y_α are Bessel functions of 1st and 2nd kind

$$Y_{i,j} = Y_{\nu_j-1}(r_0') - Y_{\nu_j+1}(r_0')$$
$$J_{i,j} = -J_{\nu_j-1}(r_0') + J_{\nu_j+1}(r_0')$$

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  - Manufacture Temperature and Ablating Surface
  - Manufacture Parameters
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Overview

- Solutions disregard boundary condition on ablating surface
- Manufacture underlying functions of ablating boundary condition
- Can manufacture arbitrary solutions without adding source term
- Much freedom, provided functions are sufficiently smooth
- Desirable properties take precedence over being physically realizable
  - Sufficient number of finite nontrivial derivatives
  - Elementary function composition

Manufacture Temperature and Ablating Surface

Manufacture $T(\mathbf{x},t)$, which requires manufacturing

- Material properties: $k(T)=\bar{k}f(T)$, $c_p(T)=\bar{c}_pf(T)$ ρ, and ϵ
  - $\bar{k}$, $\bar{c}_p$, $\rho \rightarrow \bar{\alpha}$
  - $f(T)$ relates $\theta(\mathbf{x},t)$ and $T(\mathbf{x},t)$
  - Manufacture $f(T)$ to easily compute integral $F(T)$ and its inverse $F^{-1}(\theta)$
- Transformed temperature: $\theta(\mathbf{x},t)$
  - Truncate $\theta(\mathbf{x},t)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\hat{\theta}_{i,j}(t)\varphi_{i,j}(\mathbf{x})$
  - Specify $\hat{\theta}_{i,j_0}$ in $\hat{\theta}_{i,j}(t)$
  - Specify μ_i in $u_i(x)$ and $\lambda_{i,j}$ (Cartesian) or $\lambda_{i,j}$ (polar)
- Compute temperature from $T(\mathbf{x},t)=F^{-1}(\theta(\mathbf{x},t))$

Manufacture $\mathbf{x}_s(\xi,t)$ to compute $\mathbf{n}_s(\xi,t)$ and $\dot{s}(\xi,t)$

Manufacture Parameters

Manufacture parameters to satisfy boundary condition on Γ_s:

$$-k(T_s)\frac{\partial T}{\partial n} = C_e\left[h_w(T_s, p_e) - h_r\right] + \rho\dot{s}\left[h_w(T_s, p_e) - h_s(T_s)\right] + \epsilon\sigma\left({T_s}^4 - {T_r}^4\right)$$

and recession rate:

$$\dot{s}(\xi, t) = \frac{B'(T_s, p_e)C_e}{\rho}$$

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- $\frac{\partial T}{\partial n}$, T_s, $k(T_s)$, ρ, ϵ, T_r, and $\dot{s}(\xi,t)$ already determined

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- $h_s(T_s) = h_0 + \int_{T_0}^{T_s} c_p(\hat{T})d\hat{T}$ computed from T_s and $c_p(T)$

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- Manufacture $B'(T_s, p_e)$ and $p_e(\xi, t)$

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- Manufacture $B'(T_s, p_e)$ and $p_e(\xi, t)$
- $C_e(\xi, t)$ computed from $\dot{s}(\xi, t)$, $B'(T_s, p_e)$, $p_e(\xi, t)$, and ρ

Manufacture Parameters

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and recession rate:

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- $\frac{\partial T}{\partial n}$, T_s, $k(T_s)$, ρ, ϵ, T_r, and $\dot{s}(\xi,t)$ already determined
- $h_s(T_s) = h_0 + \int_{T_0}^{T_s} c_p(\hat{T})d\hat{T}$ computed from T_s and $c_p(T)$
- Manufacture $B'(T_s,p_e)$ and $p_e(\xi,t)$
- $C_e(\xi,t)$ computed from $\dot{s}(\xi,t)$, $B'(T_s,p_e)$, $p_e(\xi,t)$, and ρ
- $h_w(T_s,p_e)$ and $h_r(\xi,t)$ need to be determined

Manufacture Parameters (continued)

Boundary condition and recession rate can be combined:

$$q_s = C_e \left(h_w(T_s, p_e) \left[1 + B'(T_s, p_e) \right] - h_r - B'(T_s, p_e) h_s(T_s) \right) + \epsilon\sigma \left(T_s^4 - T_r^4 \right)$$

- Prevent BC instabilities due to perturbations (e.g., discretization errors)
- Impose $\frac{\partial q_s}{\partial T_s} \geq 0$ so perturbations do not grow
- For radiative contribution, $\frac{\partial}{\partial T_s}(q_{s_{\text{rad.}}}) = 4\epsilon\sigma T_s^3 \geq 0$
- For non-radiative contribution, set $\frac{\partial}{\partial T_s}(q_{s_{\text{non-rad.}}}) = 0$:

$$h_w(T_s, p_e) \left[1 + B'(T_s, p_e) \right] - B'(T_s, p_e) h_s(T_s) = g(p_e)$$

$$\rightarrow h_w(T_s, p_e) = \frac{B'(T_s, p_e) h_s(T_s) + g(p_e)}{1 + B'(T_s, p_e)}$$

- Set $g(p_e) = 0$
- $h_r(\xi, t)$ can be computed since other parameters are known

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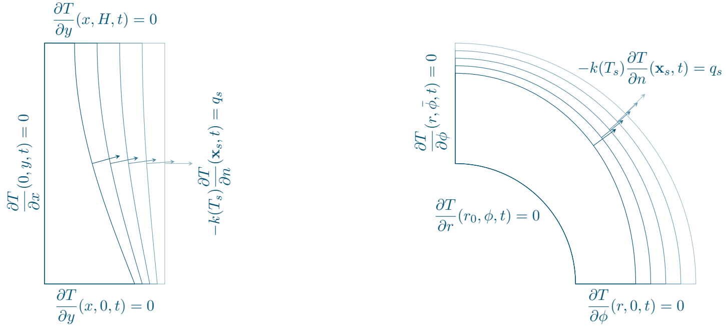
Overview



- Demonstrate methodology on two problems: Cartesian and polar
- Spatial domain discretized with $\mathcal{O}(h^2)$ finite elements
- Backward Euler time integration is $\mathcal{O}(h)$
- Each discretization doubles elements in each dimension, quarters time step
- Piecewise linear interpolation of tabulated data is $\mathcal{O}(h^2)$ – halve spacing

Error Norms

Measure error in temperature using the norm

$$\varepsilon_T = \max_{t\in[0,\bar{t}]} \|T_h(\mathbf{x},t) - T(\mathbf{x},t)\|_2$$

- L^2-norm of error computed over spatial domain
- Maximum of L^2-norms over time

Measure error in ablating surface using the norm

$$\varepsilon_{\mathbf{x}_s} = \max_{t\in[0,\bar{t}]} \|\mathbf{x}_{s_h}(\xi,t) - \mathbf{x}_s(\xi,t)\|_2$$

- L^2-norm of error computed over ablating surface

Mesh Deformation and Common Parameters

- Mesh deformation from Gent hyperelastic mesh stress model
- $\rho = 1000$ kg/m^3, $\bar{k} = 0.7$ W/m/K, $\bar{\alpha} = \{10^{-8}, 10^{-7}, 10^{-6}, 10^{-5}\}$ m^2/s $\rightarrow \bar{c}_p$
- With ($\epsilon = 0.9$) and without ($\epsilon = 0$) radiative flux
- Quartering ($\Delta t/4$) and halving ($\Delta t/2$) the time step
- Manufacture

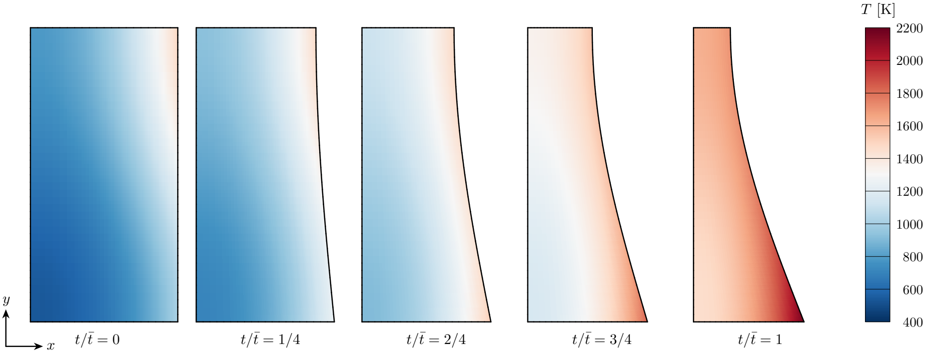
$$B'(T_s, p_e) = \exp\left(\frac{1}{1000}\frac{T_s}{\bar{T}} - \frac{1}{50}\frac{p_e}{\bar{p}}\right),$$

where $\bar{T} = 1$ K, $p_e(t) = \bar{p}e^{5t/\bar{t}}/200$, $\bar{p} = 101{,}325$ Pa, and $\bar{t} = 5$ s

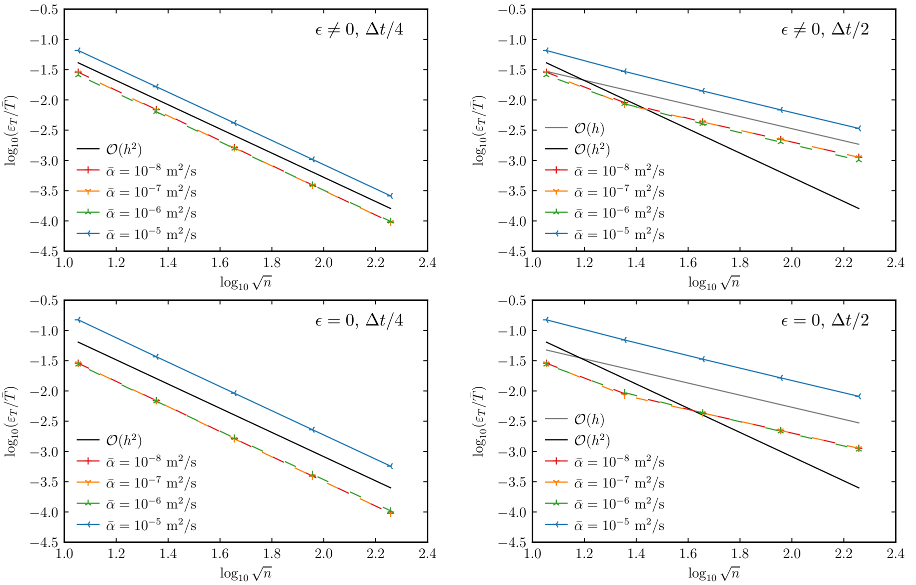
Cartesian Coordinates: Temperature and Recession

- Manufacture $f(T) = 4/3\left(T/\bar{T}\right)^{1/3} \rightarrow T(\mathbf{x},t) = F^{-1}(\theta) = \left(\bar{T}\theta(\mathbf{x},t)^3\right)^{1/4}$
  - $\bar{T} = 3000$ K
- Truncate $\theta(\mathbf{x},t) = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\hat{\theta}_{i,j}(t)\varphi_{i,j}(\mathbf{x})$ to $\max i = 0$ and $\max j = 1$
  - $v_0(y) = 1$ and $v_1(y) = \cos(\pi y/H)$ permit y variation and $\theta(\mathbf{x},t) > 0$
  - $u_0(x) = \cosh(3x/(2W))$ permits x variation and $\lambda_{i,j} < 0$
  - Set $\hat{\theta}_{0,0_0} = 400$ K and $\hat{\theta}_{0,1_0} = -100$ K
  - $\theta(\mathbf{x},t) = 100e^{22{,}500\bar{\alpha}t}\left(4 - e^{-2500\pi^2\bar{\alpha}t}\cos(\pi y/H)\right)\cosh(3x/(2W))$ K
- Manufacture $\mathbf{x}_s(\xi,t) = \left\{W\left(1 - \frac{t}{\bar{t}}\frac{1+2\sin(\pi\xi/2)}{4}\right),\ H\xi\right\}$
  - Initial domain is rectangle $\mathbf{x}_s(\xi,0) = \{W, \xi H\}$
  - ξ related to $\mathbf{x}_s$ by $\xi = y_s/H$
  - Set $W = 1$ cm, $H = 2$ cm, and $\bar{t} = 5$ s

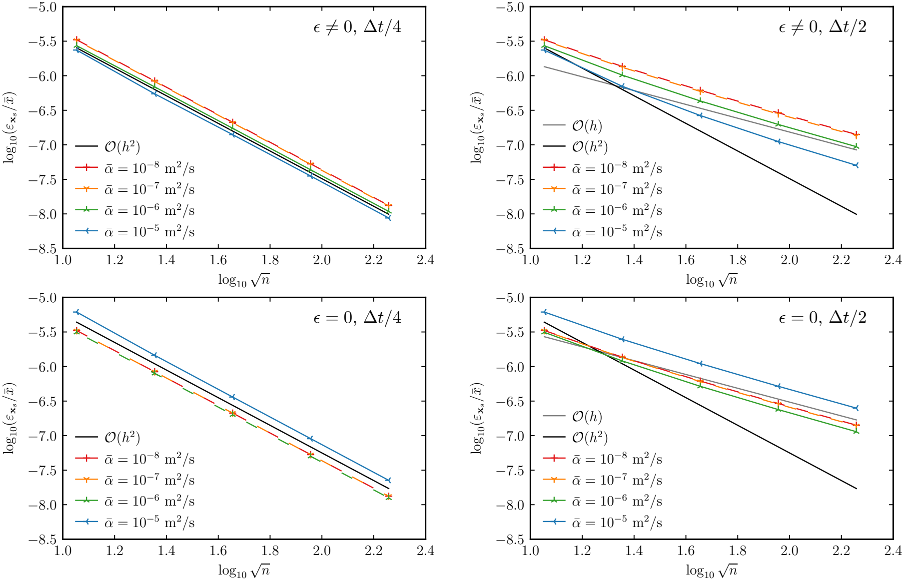
Cartesian Coordinates: Temperature and Recession ($\bar{\alpha} = 10^{-5}$ m^2/s)



Cartesian Coordinates: Norm of the Error for T



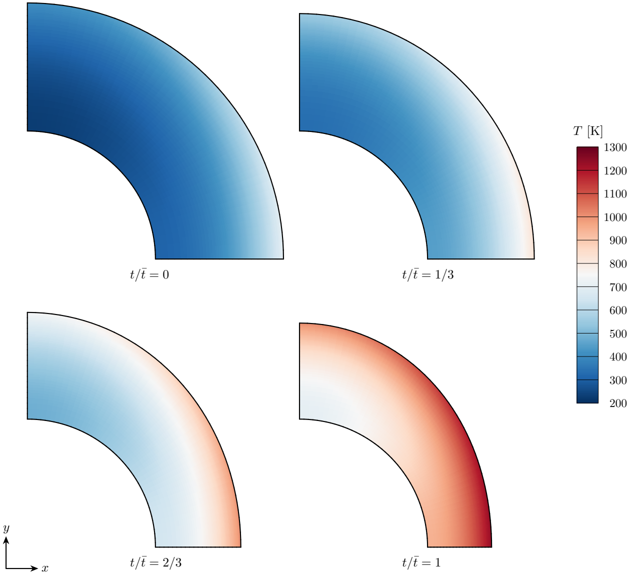
Cartesian Coordinates: Norm of the Error for $\mathbf{x}_s$



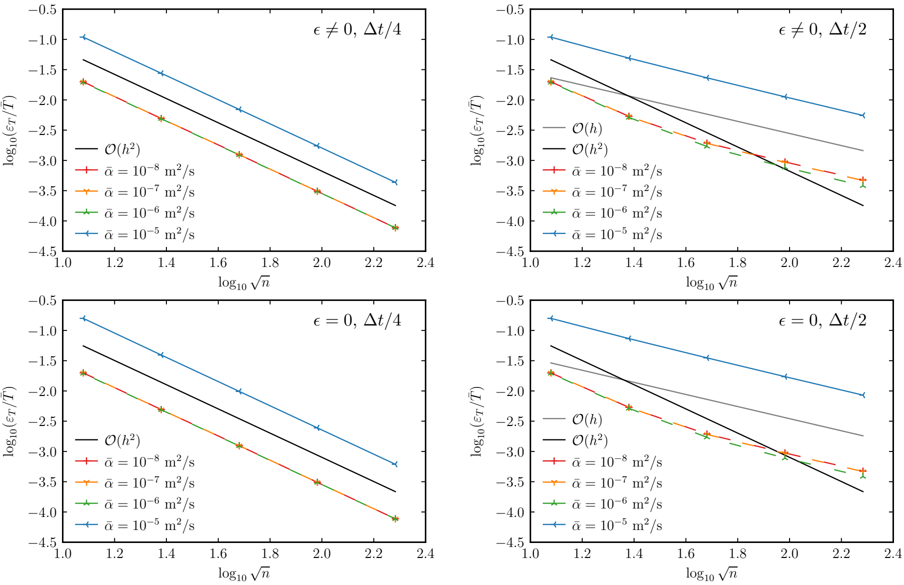
Polar Coordinates: Temperature and Recession

- Manufacture $f(T) = 1 \rightarrow T(\mathbf{x}, t) = \theta(\mathbf{x}, t)$
- Truncate $\theta(\mathbf{x}, t) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \hat{\theta}_{i,j}(t)\varphi_{i,j}(\mathbf{x})$ to $\max i = 0$ and $\max j = 1$
  - $v_0(\phi) = 1$ and $v_1(\phi) = \cos(\pi\phi/\bar{\phi})$ permit ϕ variation and $\theta(\mathbf{x}, t) > 0$
  - Set $\lambda_{0,0} = \lambda_{0,1} = -22{,}500$ m^{-2} for $u_{0,0}(r)$ and $u_{0,1}(r)$
  - Set $\hat{\theta}_{0,0_0} = 200$ K and $\hat{\theta}_{0,1_0} = 300$ K
- Manufacture $\mathbf{x}_s(\xi, t) = r_s(\xi, t)\{\cos\phi_s, \sin\phi_s\}$
  - $r_s(\xi, t) = r_1 - (r_1 - r_0)\frac{t}{\bar{t}}\frac{3+\cos(\pi\xi)}{8}$
  - Initial domain is fractional annulus $\mathbf{x}_s(\xi, 0) = r_1\{\cos\phi_s, \sin\phi_s\}$
  - ξ related to $\mathbf{x}_s$ by $\xi = \phi_s/\bar{\phi}$
  - Set $r_0 = 1$ cm, $r_1 = 2$ cm, $\bar{\phi} = \pi/2$, and $\bar{t} = 5$ s

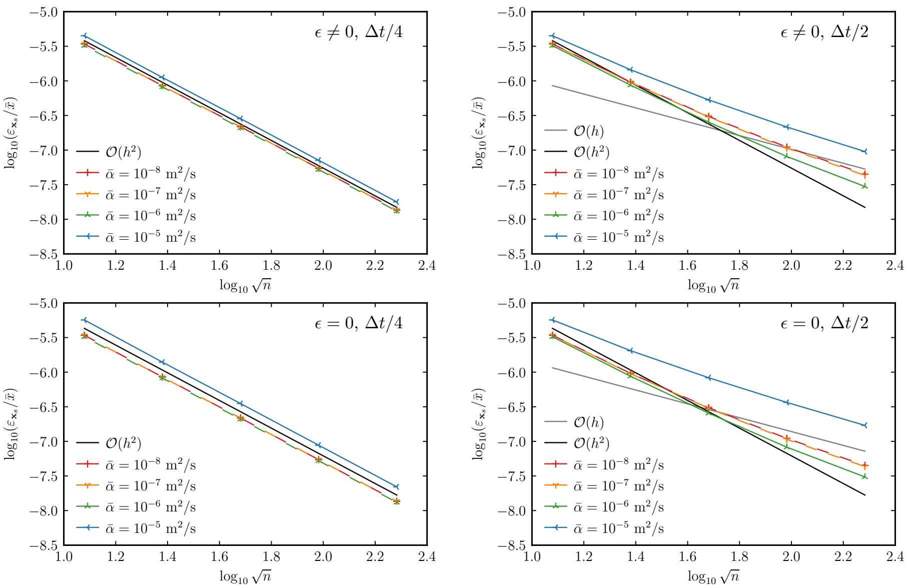
Polar Coordinates: Temperature and Recession ($\bar{\alpha} = 10^{-5}$ m^2/s)



Polar Coordinates: Norm of the Error for T



Polar Coordinates: Norm of the Error for $\mathbf{x}_s$



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Outline

- Introduction
- Governing Equations
- Manufactured Solutions
- Heat Equation Solution
- Boundary Condition Reconciliation
- Numerical Examples
- Summary
  - Code-Verification Techniques

Code-Verification Techniques

- Performed code verification for two-dimensional, non-decomposing ablation
- Derived solutions that did not require code modification
- Computed solutions to heat equations for different coordinate systems
- Manufactured boundary condition dependencies
- Demonstrated approach for two cases, which achieved expected accuracy

Additional Information

- B. Freno, B. Carnes, N. Matula
  Nonintrusive manufactured solutions for ablation
  Physics of Fluids (2021)

- B. Freno, B. Carnes, V. Brunini, N. Matula
  Nonintrusive manufactured solutions for non-decomposing ablation in two dimensions
  Journal of Computational Physics (2022) `arXiv:2110.13818`

Questions?

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