Simulation and High-Performance Computing Part 6: Method of Lines for Heat and Wave Equations

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Example: Heat equation

Model problem: Dissipation of heat in a two-dimensional domain.

$$egin{aligned} rac{\partial u}{\partial t}(t,x) &= c\Delta u(t,x) + g(t,x) \ u(t,x) &= 0 \end{aligned} \qquad ext{for all } t \in \mathbb{R}, \ x \in \Omega,$$

where u(t,x) is the temperature at time t in a point x and g(t,x) describes external heating or cooling.

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Method of lines: Replace functions by grid functions and differential operators by finite difference operators.

$$egin{aligned} rac{\partial u_h}{\partial t}(t,x) &= c\Delta_h u_h(t,x) + g(t,x) \qquad & ext{for all } t \in \mathbb{R}, \ x \in \Omega_h, \ u_h(t,x) &= 0 & ext{for all } t \in \mathbb{R}, \ x \in \partial \Omega_h. \end{aligned}$$

Reformulation as an ODE

Method of lines yields semi-discrete system

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In order to be able to apply timestepping methods, we rewrite $u_h(t,x)=u_h(t)(x)$ and obtain a system of ordinary differential equations

$$u_h'(t) = c\Delta_h u_h(t) + g_h(t)$$
 for all $t \in \mathbb{R}$

with grid functions $u_h(t) \colon \Omega_h \to \mathbb{R}$ for all $t \in \mathbb{R}$.

Adjustments: Δ_h is modified to take care of missing boundary points, and the grid functions $g_h(t) \colon \Omega_h \to \mathbb{R}$ are defined by

$$g_h(t)(x) := g(t,x)$$
 for all $t \in \mathbb{R}, x \in \Omega_h$.

Heat equation as explicit ordinary differential equation:

$$u_h(0)=u_{h,0}, \qquad u_h'(t)=c\Delta_h u_h(t)+g_h(t) \qquad \text{ for all } t\in\mathbb{R}.$$

Explicit Euler method applied to this equation yields

$$\begin{split} & ilde{u}_h(t_0) = u_{h,0}, \ & ilde{u}_h(t_{k+1}) = ilde{u}_h(t_k) + \delta(c\Delta_h ilde{u}_h(t_k) + g_h(t_k)) \end{split} \qquad ext{for all } k \in \mathbb{N}_0. \end{split}$$

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Implementation in C:

CFL condition

Eigenvectors of $-\Delta_h$: For all $\nu, \mu \in [1 : N]$, the grid function

$$e_{\nu\mu}(x) := \sin(\pi\nu x_1)\sin(\pi\mu x_2)$$
 for all $x \in \Omega_h$

satisfies

$$-\Delta_h e_{
u\mu} = \lambda_{
u\mu} e_{
u\mu}, \qquad \lambda_{
u\mu} := rac{4}{h^2} ig(\sin^2(\pi
u \, h/2) + \sin^2(\pi \mu \, h/2) ig).$$

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Explicit Euler with g=0 and $u_h(0)=e_{
u\mu}$ yields

$$\tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta c \Delta_h \tilde{u}_h(t_k) = (1 - \delta c \lambda_{\nu\mu}) \tilde{u}_h(t_k).$$

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Courant-Friedrichs-Levy condition: To avoid oscillations, we ensure

$$\delta c \, \lambda_{\nu\mu} < 1 \qquad \Longleftrightarrow \qquad \delta c \, \frac{8}{h^2} \le 1 \qquad \Longleftrightarrow \qquad \delta \le \frac{h^2}{8c}.$$

Experiment: Explicit methods for the heat equation

Approach: g=0, $u_h(0)=e_{\nu\mu}$, error measured at time t=1.

		Expl. Euler		Runge	
δ	$8c\delta/h^2$	error	ratio	error	ratio
1/16	2.1+3	1.97_{+39}		3.11_{+87}	
1/32	1.1_{+3}	4.58_{+82}		4.12_{+169}	
1/64	5.3 ₊₂	8.03_{+159}		∞	
1/16384	2.1_{+0}	∞		∞	
1/32768	1.0_{+0}	2.73_{-8}		5.49_{-12}	
1/65536	5.2_{-1}	1.36_{-8}	2.0	1.37_{-12}	4.0
1/131072	2.6_{-1}	6.83_{-9}	2.0	3.43_{-13}	4.0
1/262144	1.3_{-1}	3.41_{-9}	2.0	8.57_{-14}	4.0

Observation: No convergence while CFL condition $8c\delta/h^2 \le 1$ violated.

Implicit methods

Problem: The CFL condition forces us to use very small timesteps with explicit timestepping methods.

Implicit Euler with g=0 and $u_h(0)=e_{
u\mu}$ yields

$$egin{aligned} & ilde{u}_h(t_{k+1}) = ilde{u}_h(t_k) + \delta c \Delta_h ilde{u}_h(t_{k+1}), \ & ilde{u}_h(t_{k+1}) = rac{1}{1 + \delta c \lambda_{
u} \mu} ilde{u}_h(t_k). \end{aligned}$$

Proper exponential decay without oscillations, since $\lambda_{\nu\mu}>0$.

Crank-Nicolson with g=0 and $u_h(0)=e_{\nu\mu}$ yields

$$egin{aligned} ilde{u}_h(t_{k+1}) &= ilde{u}_h(t_k) + rac{\delta}{2}ig(c\Delta_h ilde{u}_h(t_k) + c\Delta_h ilde{u}_h(t_{k+1})ig), \ ilde{u}_h(t_{k+1}) &= \left(rac{1-rac{\delta}{2}c\lambda_{
u\mu}}{1+rac{\delta}{2}c\lambda_{
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ight) ilde{u}_h(t_k). \end{aligned}$$

Experiment: Implicit methods for the heat equation

Approach: g = 0, $u_h(0) = e_{\nu\mu}$, error measured at time t = 1.

		Impl. Euler		Crank-Nicolson	
δ	$8c\delta/h^2$	error	ratio	error	ratio
1/16	2.1_{+3}	4.46_{-3}		4.43_6	
1/32	1.1_{+3}	3.56_{-4}	12.5	2.23_{-6}	2.0
1/64	5.3_{+2}	5.33_{-5}	6.7	6.74_{-7}	3.3
1/128	2.6_{+2}	1.37_{-5}	3.9	1.77_{-7}	3.8
1/256	1.3_{+2}	4.88_{-6}	2.8	4.48_{-8}	4.0
1/512	6.6_{+1}	2.06_{-6}	2.4	1.12_{-8}	4.0
1/1024	3.3_{+1}	9.50_{-7}	2.2	2.81_{-9}	4.0
1/2048	1.7_{+1}	4.56_{-7}	2.1	7.02_{-10}	4.0

Observation: Expected convergence rates although CFL condition violated.

Example: Wave equation

Model problem: Propagation of waves in a two-dimensional domain.

$$\frac{\partial^2 u}{\partial t^2}(t,x) = c\Delta u(t,x) + g(t,x) \qquad \text{for all } t \in \mathbb{R}, \ x \in \Omega,$$
$$u(t,x) = 0 \qquad \text{for all } t \in \mathbb{R}, \ x \in \partial\Omega,$$

where u(t,x) is the displacement at time t in a point x and g(t,x) describes external forces.

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Method of lines: Replace functions by grid functions and differential operators by finite difference operators.

$$u_h''(t) = c\Delta_h u_h(t) + g_h(t)$$
 for all $t \in \mathbb{R}$.

Idea: Introduce the velocity $v_h(t) := u'_h(t)$ to obtain the familiar form

$$u_h'(t) = v_h(t),$$

$$v_h'(t) = c\Delta_h u_h(t) + g_h(t) \qquad \qquad \text{for all } t \in \mathbb{R}.$$

Explicit Euler:

$$\widetilde{u}_h(t_{k+1}) = \widetilde{u}_h(t_k) + \delta \widetilde{v}_h(t_k),
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Idea: Introduce the velocity $v_h(t) := u'_h(t)$ to obtain the familiar form

$$u_h'(t) = v_h(t),$$

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Implicit Euler: Requires us to solve two linear systems per timestep.

$$\tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta \tilde{v}_h(t_{k+1})
\tilde{v}_h(t_{k+1}) = \tilde{v}_h(t_k) + \delta c \Delta_h \tilde{u}_h(t_{k+1}) + \delta g_h(t_{k+1}).
(1 - \delta^2 c \Delta_h) \tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta \tilde{v}_h(t_k) + \delta^2 g_h(t_{k+1})
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Leapfrog:

$$\tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta \, \tilde{v}_h(t_{k+1/2}),
\tilde{v}_h(t_{k+3/2}) = \tilde{v}_h(t_{k+1/2}) + \delta \, c \Delta_h \tilde{u}_h(t_{k+1}) + \delta \, g_h(t_{k+1}).$$

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$$\begin{split} & \tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \frac{\delta}{2} \big(\tilde{v}_h(t_k) + \tilde{v}_h(t_{k+1}) \big), \\ & \tilde{v}_h(t_{k+1}) = \tilde{v}_h(t_k) + \frac{\delta}{2} c \Delta_h \big(\tilde{u}_h(t_k) + \tilde{u}_h(t_{k+1}) \big) + \frac{\delta}{2} \big(g_h(t_k) + g_h(t_{k+1}) \big). \end{split}$$

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$$\tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta \, \tilde{v}_h(t_{k+1/2}),$$

$$\tilde{v}_h(t_{k+3/2}) = \tilde{v}_h(t_{k+1/2}) + \delta \, c \Delta_h \tilde{u}_h(t_{k+1}) + \delta \, g_h(t_{k+1}).$$

$$\begin{split} \tilde{u}_h(t_{k+1}) &= \tilde{u}_h(t_k) + \frac{\delta}{2} \big(\tilde{v}_h(t_k) + \tilde{v}_h(t_{k+1}) \big), \\ \tilde{v}_h(t_{k+1}) &= \tilde{v}_h(t_k) + \frac{\delta}{2} c \Delta_h \big(\tilde{u}_h(t_k) + \tilde{u}_h(t_{k+1}) \big) + \frac{\delta}{2} \big(g_h(t_k) + g_h(t_{k+1}) \big). \\ \Big(1 - c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{u}_h(t_{k+1}) &= \Big(1 + c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{u}_h(t_k) + \delta \, \tilde{v}_h(t_k) \\ &\qquad \qquad + \frac{\delta^2}{4} \big(g_h(t_k) + g_h(t_{k+1}) \big), \\ \Big(1 - c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{v}_h(t_{k+1}) &= \Big(1 + c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{v}_h(t_k) + \delta \, c \Delta_h \, \tilde{u}_h(t_k) \\ &\qquad \qquad + \frac{\delta}{2} \big(g_h(t_k) + g_h(t_{k+1}) \big). \end{split}$$

Leapfrog:

$$\tilde{u}_h(t_{k+1}) = \tilde{u}_h(t_k) + \delta \, \tilde{v}_h(t_{k+1/2}),
\tilde{v}_h(t_{k+3/2}) = \tilde{v}_h(t_{k+1/2}) + \delta \, c \Delta_h \tilde{u}_h(t_{k+1}) + \delta \, g_h(t_{k+1}).$$

Crank-Nicolson: Requires us to solve two linear systems per timestep.

$$\begin{split} \tilde{u}_h(t_{k+1}) &= \tilde{u}_h(t_k) + \frac{\delta}{2} \big(\tilde{v}_h(t_k) + \tilde{v}_h(t_{k+1}) \big), \\ \tilde{v}_h(t_{k+1}) &= \tilde{v}_h(t_k) + \frac{\delta}{2} c \Delta_h \big(\tilde{u}_h(t_k) + \tilde{u}_h(t_{k+1}) \big) + \frac{\delta}{2} \big(g_h(t_k) + g_h(t_{k+1}) \big). \\ \Big(1 - c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{u}_h(t_{k+1}) &= \Big(1 + c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{u}_h(t_k) + \delta \, \tilde{v}_h(t_k) \\ &\qquad \qquad + \frac{\delta^2}{4} \big(g_h(t_k) + g_h(t_{k+1}) \big), \\ \Big(1 - c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{v}_h(t_{k+1}) &= \Big(1 + c \frac{\delta^2}{4} \Delta_h \Big) \, \tilde{v}_h(t_k) + \delta \, c \Delta_h \, \tilde{u}_h(t_k) \\ &\qquad \qquad + \frac{\delta}{2} \big(g_h(t_k) + g_h(t_{k+1}) \big). \end{split}$$

Experiment: Timestepping for the wave equation

Approach: g=0, $u_h(0)=e_{\nu\mu}$, $v_h(0)=0$, error measured at time t=1.

	Leapfrog		Impl. Euler		Crank-Nicol.	
δ	error	ratio	error	ratio	error	ratio
1/16	3.10_{+19}		1.07_{+2}		4.64 ₊₁	
1/32	1.63_{+33}		8.60_{+1}	1.2	1.17_{+1}	4.0
1/64	4.19_{+35}		5.50_{+1}	1.6	2.94_{+0}	4.0
1/128	3.68_{-1}		3.11_{+1}	1.8	7.36_{-1}	4.0
1/256	9.20_{-2}	4.0	1.66_{+1}	1.9	1.84_{-1}	4.0
1/512	2.30_{-2}	4.0	8.53_{+0}	1.9	4.60_{-2}	4.0
1/1024	5.75_{-3}	4.0	4.33 ₊₀	2.0	1.15_{-2}	4.0
1/2048	1.44_{-3}	4.0	2.18_{+0}	2.0	2.87_{-3}	4.0

Observation: CFL condition required for Leapfrog, but not for both implicit methods.

Reminder: The energy of the mass-spring system is conserved in the differential equation and the Crank-Nicolson method.

Energy of the wave equation:

$$\tilde{E}_h(t_k) := \tfrac{1}{2} \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle - \tfrac{c}{2} \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle.$$

Reminder: The energy of the mass-spring system is conserved in the differential equation and the Crank-Nicolson method.

Energy of the wave equation:

$$\tilde{E}_h(t_k) := \frac{1}{2} \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle - \frac{c}{2} \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle.$$

$$\begin{split} \tilde{E}(t_{k+1}) - E(t_k) &= \frac{1}{2} \left(\langle \tilde{v}_h(t_{k+1}), \tilde{v}_h(t_{k+1}) \rangle - \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle \right) \\ &- \frac{c}{2} \left(\langle \tilde{u}_h(t_{k+1}), \Delta_h \tilde{u}_h(t_{k+1}) \rangle - \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle \right) \end{split}$$

Reminder: The energy of the mass-spring system is conserved in the differential equation and the Crank-Nicolson method.

Energy of the wave equation:

$$\tilde{E}_h(t_k) := \frac{1}{2} \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle - \frac{c}{2} \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle.$$

$$\begin{split} \tilde{E}(t_{k+1}) - E(t_k) &= \frac{1}{2} \left(\langle \tilde{v}_h(t_{k+1}), \tilde{v}_h(t_{k+1}) \rangle - \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle \right) \\ &- \frac{c}{2} \left(\langle \tilde{u}_h(t_{k+1}), \Delta_h \tilde{u}_h(t_{k+1}) \rangle - \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle \right) \\ &= \frac{1}{2} \langle \tilde{v}_h(t_{k+1}) - \tilde{v}_h(t_k), \tilde{v}_h(t_{k+1}) + \tilde{v}_h(t_k) \rangle \\ &- \frac{c}{2} \langle \tilde{u}_h(t_{k+1}) - \tilde{u}_h(t_k), \Delta_h (\tilde{u}_h(t_{k+1}) + \tilde{u}_h(t_k)) \rangle \end{split}$$

Reminder: The energy of the mass-spring system is conserved in the differential equation and the Crank-Nicolson method.

Energy of the wave equation:

$$\tilde{E}_h(t_k) := \frac{1}{2} \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle - \frac{c}{2} \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle.$$

$$\begin{split} \tilde{E}(t_{k+1}) - E(t_k) &= \frac{1}{2} \left(\left\langle \tilde{v}_h(t_{k+1}), \tilde{v}_h(t_{k+1}) \right\rangle - \left\langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \right\rangle \right) \\ &- \frac{c}{2} \left(\left\langle \tilde{u}_h(t_{k+1}), \Delta_h \tilde{u}_h(t_{k+1}) \right\rangle - \left\langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \right\rangle \right) \\ &= \frac{1}{2} \left\langle \tilde{v}_h(t_{k+1}) - \tilde{v}_h(t_k), \tilde{v}_h(t_{k+1}) + \tilde{v}_h(t_k) \right\rangle \\ &- \frac{c}{2} \left\langle \tilde{u}_h(t_{k+1}) - \tilde{u}_h(t_k), \Delta_h(\tilde{u}_h(t_{k+1}) + \tilde{u}_h(t_k)) \right\rangle \\ &= \delta \frac{c}{4} \left\langle c \Delta_h(\tilde{u}_h(t_k) + \tilde{u}_h(t_{k+1})), \tilde{v}_h(t_{k+1}) + \tilde{v}_h(t_k) \right\rangle \\ &- \delta \frac{c}{4} \left\langle \tilde{v}_h(t_k) + \tilde{v}_h(t_{k+1}), \Delta_h(\tilde{u}_h(t_{k+1}) + \tilde{u}_h(t_k)) \right\rangle \end{split}$$

Reminder: The energy of the mass-spring system is conserved in the differential equation and the Crank-Nicolson method.

Energy of the wave equation:

$$\tilde{E}_h(t_k) := \frac{1}{2} \langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \rangle - \frac{c}{2} \langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \rangle.$$

$$\begin{split} \tilde{E}(t_{k+1}) - E(t_k) &= \frac{1}{2} \left(\left\langle \tilde{v}_h(t_{k+1}), \tilde{v}_h(t_{k+1}) \right\rangle - \left\langle \tilde{v}_h(t_k), \tilde{v}_h(t_k) \right\rangle \right) \\ &- \frac{c}{2} \left(\left\langle \tilde{u}_h(t_{k+1}), \Delta_h \tilde{u}_h(t_{k+1}) \right\rangle - \left\langle \tilde{u}_h(t_k), \Delta_h \tilde{u}_h(t_k) \right\rangle \right) \\ &= \frac{1}{2} \left\langle \tilde{v}_h(t_{k+1}) - \tilde{v}_h(t_k), \tilde{v}_h(t_{k+1}) + \tilde{v}_h(t_k) \right\rangle \\ &- \frac{c}{2} \left\langle \tilde{u}_h(t_{k+1}) - \tilde{u}_h(t_k), \Delta_h(\tilde{u}_h(t_{k+1}) + \tilde{u}_h(t_k)) \right\rangle \\ &= \delta \frac{c}{4} \left\langle c \Delta_h(\tilde{u}_h(t_k) + \tilde{u}_h(t_{k+1})), \tilde{v}_h(t_{k+1}) + \tilde{v}_h(t_k) \right\rangle \\ &- \delta \frac{c}{4} \left\langle \tilde{v}_h(t_k) + \tilde{v}_h(t_{k+1}), \Delta_h(\tilde{u}_h(t_{k+1}) + \tilde{u}_h(t_k)) \right\rangle = 0. \end{split}$$

Summary

Method of lines: Discretize in space to obtain a system of coupled ordinary differential equations. \rightarrow Solve by timestepping methods.

Heat equation: Explicit methods require the CFL condition, i.e., the stepsize δ has to be quite small.

Implicit methods can avoid this requirement, but require us to solve a linear system in each step.

Wave equation: Explicit methods require the CFL condition, implicit methods can avoid it, but require us to solve two linear systems each step. Crank-Nicolson method conserves the energy.