Advanced Intro to CFD – HW5

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1 Introduction

The 1D unsteady heat equation was solved using a second-order accurate explicit discretization in space and a first-order accurate explicit time scheme. The 1D heat equation is

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = f(x), \tag{1}$$

where α, the thermal diffusivity, is $9.71 \times 10^{-5}\,\mathrm{m}^2/\mathrm{s}$, and $f(x)$ is a source term for the particular problem at hand. The explicit discretization implemented is

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} - \alpha \frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x} = f(x_i), \tag{2}$$

where i is node number and n is the current time iteration. This was solved using local time stepping until the maximum number of iterations reached (100 000 to 400 000 iterations) or the relative iterative residual (using the 2-norm) dropped below 1×10^{-9}.

2 Part 1

The first goal is to check the solver implementation using a steady-state manufactured solution. This solution is given by

$$T(x) = 300 + 200 \sin\left(\frac{3\pi x}{2L}\right) \mathrm{K},\ L = 1\mathrm{m}, \tag{3}$$

where L is the length of the bar and x is the current position along the bar. This solution is used in the governing equation, with the time derivative term ignored, to determine the required source term. Solving for the second derivative of temperature, and plugging the value into equation (1), the source term becomes

$$f(x) = \frac{450\pi^2}{\alpha L^2} \sin\left(\frac{3\pi x}{2L}\right). \tag{4}$$

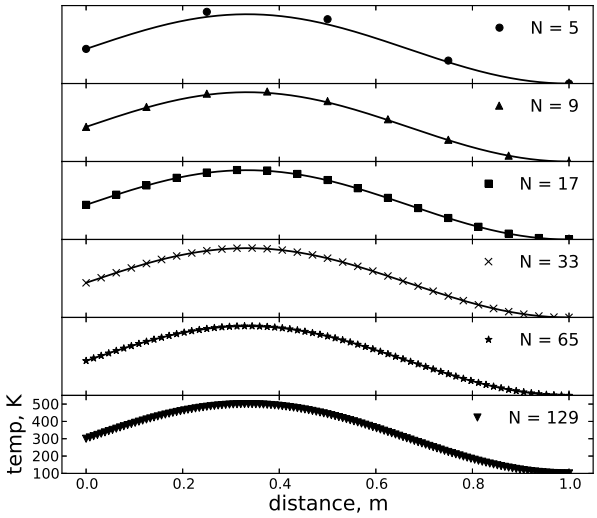


Figure 1: Temperature solution with exact solution overlaid.

The manufactured problem was solved on six different grids with a grid refinement fact, h, of two for each successive grid. Nodes were evenly-spaced with grids of 5, 9, 17, 33, 65 and 129 nodes in the domain $0 \leq x \leq 1$m. The boundary conditions were determined from the temperature solution (Eq. 3) and are 300 K and 100 K on the left and right boundaries, respectively.

At each iteration, the steady-state iterative convergence was examined by taking both the L_∞ and L_2 norms. The relative iterative residual, calculated by normalizing the iterative residual by the first iterative residual, was used as the criterion to exit the time stepping loop. The steady-state iterative residual is

$$R_i^n = \alpha \frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x} + f(x_i). \tag{5}$$

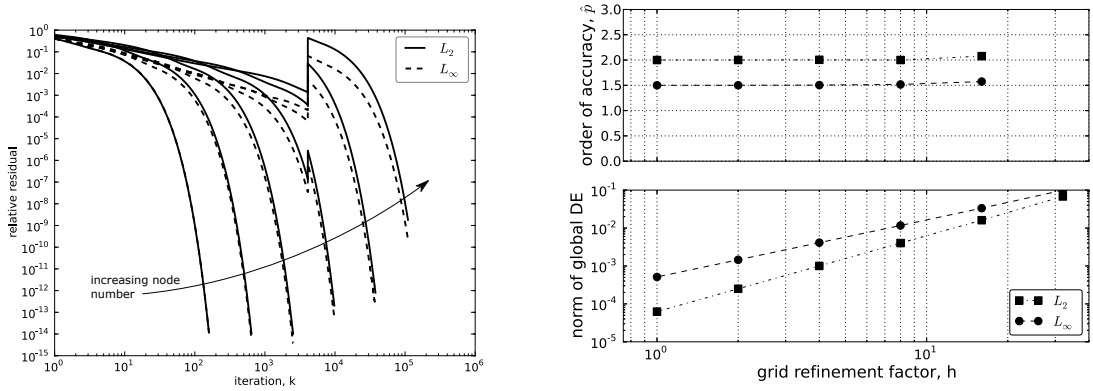
The observed order of accuracy was also calculated using a coarse and fine mesh. It is found using

$$\hat{p} = \frac{\ln(DE_2)/DE_1}{\ln r}, \tag{6}$$

where DE_2 and DE_1 are the discretization errors for the coarse and fine meshes, respectively, and r is the grid refinement factor (which is two for the current study).

2.1 Results

Temperature profiles for the manufactured solution and exact solution overlaid is shown if figure 1. As expected, the finest grid most faithfully represents the exact solution.



(a) Residuals

(b) Order of accuracy

Figure 2: Relative iterative residuals and order of accuracy for the manufactured solution.

The relative iterative residuals for the different node numbers and order of accuracy calculations are shown in figure 2a and figure 2b, respectively. The finer grids should have been run longer to reach a lower iterative error, but the solution is still close. The observed order of accuracy, $\hat{p}$, is two when calculated using L_2 and 1.5 when using L_∞. This method should be second order accurate, and it is.

3 Part 2

The goal of part 2 is to solve the 1D unsteady heat equation, like part 1, but with a different source term and not using the method of manufactured solutions. The source term is

$$f(x) = 100 \left[0.25 \left(0.75 - \left| x - \frac{2}{3} \right| \right) \right]^4 \text{ K/s}. \tag{7}$$

The bar is initially at a uniform temperature of 300 K, with a constant temperature boundary condition of 300 K at $x = 0$ and a temperature derivative of -200 K/m at $x = 1$. This problem was solved with local time stepping to the steady-state solution, like in part 1, except that first- and second-order explicit schemes were used to determine the temperature at the right boundary (and compare how both perform). The temperature at T^n_{i-1} and T^n_{i-2} were expanded in a Taylor series about the end wall point as follows:

$$T^n_{i-1} = T^n_i + \left.\frac{\partial T}{\partial x}\right|^n_i (-\Delta x) + \left.\frac{\partial^2 T}{\partial^2 x}\right|^n_i \frac{(-\Delta x)^2}{2} + \mathcal{O}(\Delta x^3) \tag{8}$$

$$T^n_{i-2} = T^n_i + \left.\frac{\partial T}{\partial x}\right|^n_i (-2\Delta x) + \left.\frac{\partial^2 T}{\partial^2 x}\right|^n_i \frac{(-2\Delta x)^2}{2} + \mathcal{O}(\Delta x^3). \tag{9}$$

For the first-order accurate scheme, eq. (8) is rearranged for T_i^n as

$$T_i^n = T_{i-1}^n + \left.\frac{\partial T}{\partial x}\right|_i^n + \mathcal{O}(\Delta x^2). \tag{10}$$

For the second order accurate scheme, we combine eqns. (8) and (9) such that the second-terms cancel. We subtract 4(9) from (8) and rearrange to get

$$T_i^n = \frac{1}{3}\left[4T_{i-1}^n - T_{i-2}^n + 2\Delta x \left.\frac{\partial T}{\partial x}\right|_i^n\right] + \mathcal{O}(\Delta x^3). \tag{11}$$

The above equations were used to solve for the temperature at the boundary after all of the interior nodes had been solved for.

Additionally, for part 2, the Grid Convergence Index (GCI) was used to estimate the numerical uncertainty in the steady-state solution. The GCI is define as

$$GCI = \frac{F_s}{r^p - 1}\left|\frac{f_2 - f_1}{f_1}\right|, \tag{12}$$

where F_s is a factor of safety (3 was used for this study), r is the refinement factor from going from the coarse (subscript 2) to fine (subscript 1) grids, p is the order of accuracy of the numerical scheme, and f is the numerical solution at the different node locations for the different grids. Note that this assumes one is in the asymptotic regime, which can be checked by observing the iterative residual plot.

3.1 Results

The temperature profiles for using both the first- and second-order is shown in figure 3. The second order accurate scheme converges to the correct value sooner with a smaller grid than the first order accurate method, which is expected. Additionally, the first order method under-predicts the temperature profile, while the second-order scheme over-predicts.

The iterative relative residual using both schemes is shown in figure 4a and the GCI is shown in figure 4b. The fine grid does not reach the residual cutoff of 1×10^{-12}, but it is close after 400 000 iterations. The GCI does a good job of showing the difference between the first- and second- order accurate schemes. The finest grid using the first-order method is only slightly better than the second coarsest grid using the second-order method.

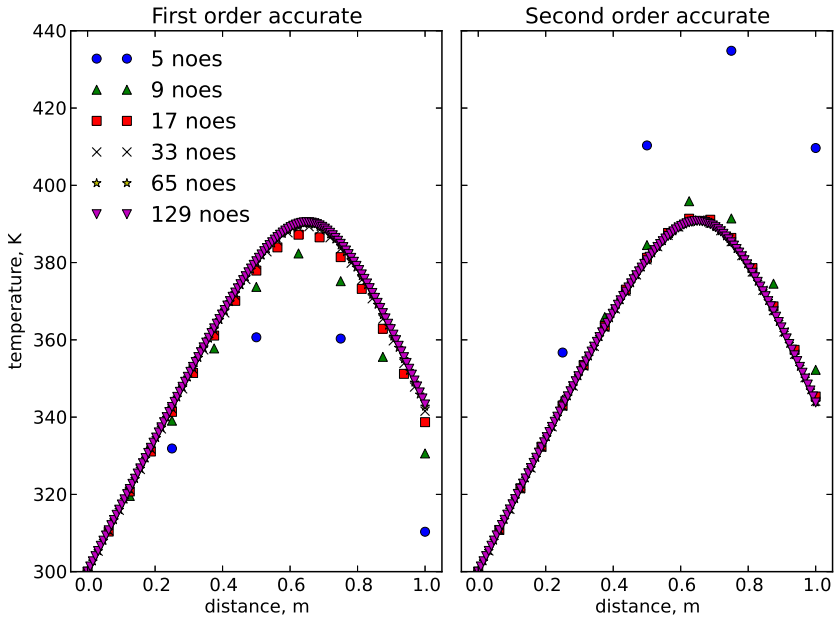
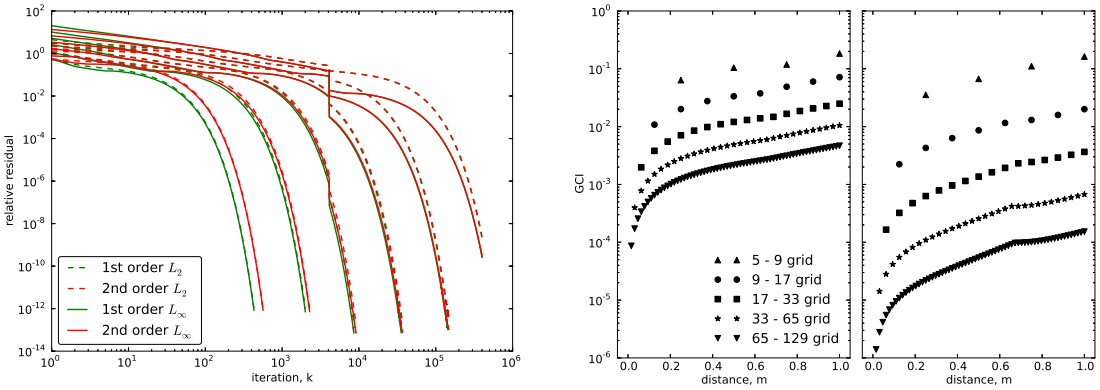


Figure 3: Temperature profiles for different meshes and using first and second order accurate scheme to find the temperature at $x = 1$.



(a) Relative residuals

(b) Grid convergence index

Figure 4: Temperature solution for first- and second-order accuate scheme.

4 Code and implementation

The source code for this was written in an IPython notebook, which is available at `https://github.com/isaacyeaton/adv-intro-cfd-2012`. A pdf version of this notebook is attached below, but an html version is available on the Github page as `hw5.html`.

1 Common functions

```
def grid_pts(ngrid, x0=0, x1=1):
    """Return evenly spaced grid points over the given interval.

    Inputs:
        ngrid (int) - number of grid points
        x0 (float, optional) - start of grid
        x1 (float, optional) - end of grid

    Outputs:
        grid (array of floats) - vector of grid points
        dx (float) - grid spacing
    """

    grid = np.linspace(x0, x1, ngrid)
    assert np.allclose(x0, grid[0])
    assert np.allclose(x1, grid[-1])
    dx = np.diff(grid)[0]

    return grid, dx


def ooa(de2, de1, r=2.):
    """Observed order of accuracy.

    Inputs:
        de2 (float) - DE error of coarse mesh
        de1 (float) - DE error of fine mesh
        r (float, default=2.) - grid refinement factor

    Outputs:
        phat (float) - observed order of accuracy
    """

    return np.log(de2 / de1) / np.log(r)


def find_phat(DE, r=2.):
    """Find the observed order of accuracy.

    Inputs:
        DE (array) - discretization error using L2 and Linf norms
        r (float, default=2.) - refinement factor

    Outputs:
        phat (array) - observed order of accuracy
    """

    npts = len(DE) - 1
    phat = np.zeros((npts, 2))
```

```
    for i in range(npts):
        phat[i] = ooa(DE[i, 0], DE[i+1, 0], r=r), ooa(DE[i, 1], DE[i+1, 1], r=r)

    return phat


def find_h(grids):
    """Find the normalized grid spacing 'h'.

    Inputs:
        grids (array) - possible grid shapes, from smallest to largest

    Outputs:
        h (array, int) - normalized grid spacing.
    """

    dx = np.zeros(grids.shape)
    for i, ngrid in enumerate(grids):
        _, dx[i] = grid_pts(ngrid)
    h = dx / dx[-1]

    return h.astype(np.int)


def find_gci(d2, d1, p, Fs=3, r=2):
    """Grid Convergence Index using Roache (1994) method.

    Inputs:
        x2 (array) - grid of the coarse mesh
        x1 (array) - grid of the fine mesh
        f2 (array) - solution on coarse mesh
        f1 (array) - solution on fine meash
        p (float) - order of accuracy
        FS (default=3) - factor of safety
        r (default=2) - grid refinement factor

    Outputs:
        gci (float) - grid convergence index of fine grid
    """

    x2, f2 = d2[:, 0], d2[:, 1]
    x1, f1 = d1[:, 0], d1[:, 1]

    assert len(f1) > len(f2)
    assert len(x2) == len(f2)
    assert len(x1) == len(x1)

    # common grid points for both meshes
    f1_mask = np.in1d(x1, x2)

    c = np.float(Fs) / (r**p - 1)
```

```
    gci = c * np.abs((f2 - f1[f1_mask]) / f1[f1_mask])

    return x2, gci
```

2 Perform a code validation study

Peform a code validation study using the steady-state manufactured soluation given by

$$T(x) = 300 + 200 \sin\left(\frac{3\pi x}{2L}\right) K,\ L = 1m$$

```
def exact_p1(x, L=1):
    """Exact solution for verification."""

    return 300. + 200. * np.sin(3 * np.pi * x / (2 * L))


def source_p1(x, alpha, L=1):
    """Source term for manufactured solution."""

    return 450. * alpha * (np.pi / L) ** 2 * np.sin(3*np.pi*x / (2*L))


def solver_p1(T, f, c, dt, kmax):
    """Solver for 1D unsteady heat equation.

    Inputs:
        T (array) - temperature array at inital value
        f (array) - source term evaluated at grid points
        c (float) - alpha / dx**2
        dt (float) - time step
        kmax (int) - max number of iterations to perfom

    Returns:
        T (array) - numerical solution
        L (array) - L2 and Linf of the relative iterative residuals
    """

    assert len(T) == len(f)
    ngrid = len(f)
    imin, imax = 1, ngrid - 1
    Rtmp = 1.

    R = np.zeros(ngrid)
    L = np.zeros((kmax, 2))

    for k in range(kmax):

        # steady-state iterative residual
        for i in range(imin, imax):
            R[i] = c * (T[i-1] - 2*T[i] + T[i+1]) + f[i]
```

```
        Rtmp = norm(R)
        L[k] = Rtmp, norm(R, np.inf)

        # update the temperature value
        T = T + dt * R
        T[0], T[-1] = 300., 100.

        if Rtmp / L[0, 0] <= 1e-14:
            break

    L /= L[0]

    return T, L[:k]
```

```
kmax = 110000
x0, x1 = 0, 1
alpha = 9.71e-5
poss_grids = np.array([5, 9, 17, 33, 65, 129])

namet = './data/MMS_{0}_{1}.npy'
Tnames, Lnames = [], []
save_files = False
```

```
for ngrid in poss_grids:

    x, dx = grid_pts(ngrid)
    dt = .3 * dx**2 / alpha
    c = alpha / dx**2

    f = source_p1(x, alpha)
    T = 300. * np.ones(ngrid)
    T[0], T[-1] = exact_p1(x0), exact_p1(x1)

    start = time.time()
    T, L = solver_p1(T, f, c, dt, kmax)
    print('{0} grid pts: {1:.2f} sec'.format(ngrid, time.time() - start))

    if save_files:
        Tname = namet.format(ngrid, 'T')
        Lname = namet.format(ngrid, 'L')
        Tnames.append(Tname)
        Lnames.append(Lname)
        np.save(Tname, np.c_[x, exact(x), T])
        np.save(Lname, L)

pickle.dump([Tnames, Lnames], open('./data/MSM_names', 'wb'))
```

2.1 Make plots of solution and relative iterative residual

```
fig1, ax = plt.subplots(6, 1, sharex=True)
fig2, ax2 = plt.subplots()

Tnames, Lnames = pickle.load(open('./data/MSM_names', 'rb'))
markers = ['o', '^', 's', 'x', '*', 'v']
xx = np.linspace(0, 1, 1000)
ex = exact_p1(xx)
DE = np.zeros((len(Tnames), 2))

for i in range(len(Tnames)):

    Tf, Lf = Tnames[i], Lnames[i]
    grid = str(poss_grids[i])

    T, L = np.load(Tf), np.load(Lf)
    de = (T[:, 2] - T[:, 1]) / T[:, 1]
    DE[i] = norm(de, np.inf), norm(de, 2)

    ax[i].plot(T[:, 0], T[:, 2], color='k', ls='None', marker=markers[i], label='N = {0}'
        .format(grid))
    ax[i].plot(xx, ex, '-k', lw=1.5, alpha=.75)
    ax[i].set_yticks(np.arange(100, 600, 100))
    ax[i].set_xlim(-0.05, 1.05)
    ax[i].legend(loc='upper right', frameon=False, numpoints=1)

    ax2.loglog(L[:, 0], 'k', lw=2)
    ax2.loglog(L[:, 1], '--k', lw=2)
    #ax2.semilogy(L[:, 0], 'k', lw=2)
    #ax2.semilogy(L[:, 1], '--k', lw=2)

for axis in ax[:-1]:
    axis.set_yticks([])

ax[-1].set_xlabel('distance, m', fontsize='x-large')
ax[-1].set_ylabel('temp, K', fontsize='x-large')
ax[-1].tick_params(axis='x', which='major', labelsize=12)
fig1.subplots_adjust(bottom=.08, top=.99, hspace=0)

ax2.set_ylabel('relative residual')
ax2.set_xlabel('iteration, k')
leg = ax2.legend((r'$L_2$', r'$L_\infty$'), loc='best', fancybox=True)
leg.get_frame().set_alpha(0.5)

#ax2.annotate('0.25 on data', (1e3, 1e-13), textcoords='data', size=10)

#fig1.savefig('./report/figs/MMS_profiles.eps')
#fig2.savefig('./report/figs/MMS_resid.eps')
#fig2.savefig('./report/figs/MMS_resid.svg')
```

```
# find order of accuracy and normalized grid spacing
phat = find_phat(DE)
h = find_h(poss_grids)


fig, (ax1, ax2) = plt.subplots(2, 1, sharex=True)

ax1.semilogx(h[1:], phat[:, 0], '-.ks', ms=8, label=r'$L_2$')
ax1.semilogx(h[1:], phat[:, 1], '--ko', ms=8, label=r'$L_\infty$')
ax1.grid(True, which='both')

ax1.set_ylim(0, 3)
ax1.set_ylabel(r'order of accuracy, $\hat{p}$', fontsize='x-large')
ax1.tick_params(axis='both', which='major', labelsize=14)

ax2.loglog(h, DE[:, 0], '-.ks', ms=8, label=r'$L_2$')
ax2.loglog(h, DE[:, 1], '--ko', ms=8, label=r'$L_\infty$')
ax2.grid(True, axis='x', which='both')
ax2.tick_params(axis='both', which='major', labelsize=14)

ax2.set_xlim(.75, 40)
ax2.set_xlabel('grid refinement factor, h', fontsize='x-large')
ax2.legend(loc='lower right', fancybox=True)
ax2.set_ylabel(r'norm of global DE', fontsize='x-large')

fig.tight_layout()

fig.savefig('./report/figs/MMS_ooa.eps')

#hh = np.linspace(.01, 40, 1000)
#offset = -1e-5
#ff = 1 * hh - offset
#ss = 2 * hh - offset
#ax.loglog(hh, ff)
#ax.loglog(hh, ss)
```

3 Part 2

Numerical solution for the heated bar with a source term.

```
def source_p2(x):
    """Source term for part 2."""

    return 100 * (.25 * (.75 - np.abs(x - 2./3))) ** 4


def solver_p2(T, f, c, dt, kmax, BC=1):
    """Solver for 1D unsteady heat equation.

    Inputs:
        T (array) - temperature array at inital value
```

```
        f (array) - source term evaluated at grid points
        c (float) - alpha / dx**2
        dt (float) - time step
        kmax (int) - max number of iterations to perfom

    Returns:
        T (array) - numerical solution
        L (array) - L2 and Linf of the relative iterative residuals
    """

    assert len(T) == len(f)
    ngrid = len(f)
    imin, imax = 1, ngrid - 1
    Rtmp = 1.
    Tbc = -200 # K/m

    R = np.zeros(ngrid)
    L = np.zeros((kmax, 2))

    for k in range(kmax):

        # steady-state iterative residual
        for i in range(imin, imax):
            R[i] = c * (T[i-1] - 2*T[i] + T[i+1]) + f[i]
        Rtmp = norm(R)
        L[k] = Rtmp, norm(R, np.inf)

        # update the temperature value
        T = T + dt * R

        # update the derivative boundary condition
        if BC == 1:
            T[-1] = T[-2] + dx * Tbc
        elif BC == 2:
            T[-1] = 1/3. * (4*T[-2] - T[-3] + 2*dx*Tbc)

        if Rtmp / L[0, 0] <= 1e-12:
            break

    L /= L[0]

    return T, L
```

```
kmax = 400000
x0, x1 = 0, 1
alpha = 9.71e-5
poss_grids = np.array([5, 9, 17, 33, 65, 129])
bcs = np.array([1, 2])

x, dx = grid_pts(ngrid)
dt = .3 * dx**2 / alpha
```

```
c = alpha / dx**2

namet = './data/p2_{0:03d}_{1}_BC{2}.npy'
save_files = False
```

```
for ngrid in poss_grids:
    for BC in bcs:
        x, dx = grid_pts(ngrid)
        dt = .3 * dx**2 / alpha
        c = alpha / dx**2

        f = source_p2(x)
        T = 300. * np.ones(ngrid)

        start = time.time()
        T, L = solver_p2(T, f, c, dt, kmax, BC=BC)
        print('{0} grid pts: {1:.2f} sec'.format(ngrid, time.time() - start))

        if save_files:
            Tname = namet.format(ngrid, 'T', BC)
            Lname = namet.format(ngrid, 'L', BC)
            np.save(Tname, np.c_[x, T])
            np.save(Lname, L)
```

```
129 grid pts: 126.91 sec
129 grid pts: 129.80 sec
```

```
BC1_T = sorted(glob('./data/*T_BC1*'))
BC2_T = sorted(glob('./data/*T_BC2*'))
BC1_L = sorted(glob('./data/*L_BC1*'))
BC2_L = sorted(glob('./data/*L_BC2*'))
nruns = len(BC1_T)

fig1, ax = plt.subplots(1, 2, sharex=True, sharey=True)
fig2, ax2 = plt.subplots()

markers = ['o', '^', 's', 'x', '*', 'v']
colors = ['b', 'g', 'r', 'k', 'y', 'm']
DE_1 = np.zeros((nruns, 2))
DE_2 = DE_1.copy()


for i in range(nruns):

    grid = poss_grids[i]
    t1, t2 = np.load(BC1_T[i]), np.load(BC2_T[i])
    l1, l2 = np.load(BC1_L[i]), np.load(BC2_L[i])
```

```
    ax[0].plot(t1[:, 0], t1[:, 1], ls='None', color=colors[i], ms=6, marker=markers[i],
        alpha=.75, label='{0} noes'.format(grid))
    ax[1].plot(t2[:, 0], t2[:, 1], ls='None', color=colors[i], ms=6, marker=markers[i],
        alpha=.75)

    if True:
        lw = 1.5
        ax2.loglog(l1[:, 0], 'g--', lw=lw)
        ax2.loglog(l2[:, 0], 'r--', lw=lw)
        ax2.loglog(l1[:, 1], 'g', lw=lw)
        ax2.loglog(l2[:, 1], 'r', lw=lw)

ax[0].set_title('First order accurate')
ax[1].set_title('Second order accurate')
ax[0].legend(loc='best', frameon=False)
ax[0].set_xlabel('distance, m')
ax[1].set_xlabel('distance, m')
ax[0].set_ylabel('temperature, K')
ax[0].set_xlim(-0.05, 1.05)
ax[0].tick_params(axis='both', which='major', labelsize=12)

ax2.set_ylabel('relative residual')
ax2.set_xlabel('iteration, k')
ax2.tick_params(axis='both', which='major', labelsize=12)
leg = ax2.legend((r'1st order $L_2$', r'2nd order $L_2$', r'1st order $L_\infty$', r'2nd
    order $L_\infty$'), loc='best', fancybox=True)
leg.get_frame().set_alpha(0.5)

fig1.subplots_adjust(hspace=0)
fig1.tight_layout()
#fig1.savefig('./report/figs/p2_profiles.eps')

fig2.tight_layout()
#fig2.savefig('./report/figs/p2-relresid.eps')
```

```
fig, (ax1, ax2) = plt.subplots(1, 2, sharex=True, sharey=True)
markers = ['^', 'o', 's', '*', 'v']

for i in range(nruns - 1):

    grid_h2, grid_h1 = poss_grids[i], poss_grids[i+1]
    t1_h1, t2_h1 = np.load(BC1_T[i]), np.load(BC2_T[i])
    t1_h2, t2_h2 = np.load(BC1_T[i+1]), np.load(BC2_T[i+1])

    gcix1, gci1 = find_gci(t1_h1, t1_h2, 1)
    gcix2, gci2 = find_gci(t2_h1, t2_h2, 2)

    label = '{0} - {1} grid'.format(grid_h2, grid_h1)
    ax1.semilogy(gcix1, gci1, 'k', ls='None', marker=markers[i], label=label)
    ax2.semilogy(gcix2, gci2, 'k', ls='None', marker=markers[i])
```

```
ax1.legend(loc='lower right', frameon=False, numpoints=2)
ax1.set_xlabel('distance, m')
ax2.set_xlabel('distance, m')
ax1.set_xlim(-.05, 1.05)
ax2.set_xlim(-.05, 1.05)
ax1.set_ylabel('GCI')

fig.tight_layout()

#fig.savefig('./report/figs/p2_gci.eps')
```