Global communications in multiprocessor simulations of flames

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Abstract

In this paper we investigate performance of global communications in a particular parallel code. The code simulates dynamics of expansion of premixed spherical flames using an asymptotic model of Sivashinsky type and a spectral numerical algorithm. As a result, the code heavily relies on global all-to-all interprocessor communications implementing transposition of the distributed data array in which numerical solution to the problem is stored. This global data interdependence makes interprocessor connectivity of the HPC system as important as the floating-point power of the processors of which the system is built. Our experiments show that efficient numerical simulation of this particular model, with global data interdependence, on modern HPC systems is possible. Prospects of performance of more sophisticated models of flame dynamics are analysed as well.

Keyword: Global interprocessor communications, distributed array transposition, premixed spherical flames
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1 Introduction

The problem under consideration stems from the studies of dynamics of premixed flames affected by the hydrodynamic flame instability. These flames

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are common in science and engineering applications, in particular in working out industrial safety requirements in petrochemical plants, in design of internal combustion engines, and in astrophysics. Expanding spherical flames are one of the most important types of premixed flames and are a popular subject of fundamental and applied studies. In particular, a possibility of a self-induced transition from deflagration to detonation is the issue of a great importance both in practice and theory.

One of the most distinctive features of these flames is that their expansion rate does not remain constant, as one would expect, but it grows in proportion to the square root of time [1]. Theoretical evaluations indicate that the expansion rate should depend on physical dimension of the problem and numerical simulations confirmed this for planar circular flames, see e.g. [2] and references therein. Calculations of spherical flames carried out so far, using an asymptotic Sivashinsky type model, remain inconclusive, because it was impossible to cover long enough time intervals to allow flames to stabilize to the asymptotic power-law regime [3]. The direct three-dimensional Navier-Stokes simulations do not look feasible at present at all, because long time intervals mean large flame radii, i.e. large Reynolds numbers.

Mathematical model used in our simulations needs intensive all-to-all data exchanges and, as a result, the scalability of our MPI code is expected to degrade as the number of processors brought into play grows. Extrapolation of the code performance has indicated that the computer resources needed to carry out the calculations until stabilization of flames to the asymptotic power-law regime may require up to a few processor-years. On the other hand, reaching this asymptotic power-law regime of expansion of spherical flames numerically is crucial in order to justify studies of pseudoresonant interaction of flame wrinkles with the upstream velocity perturbations [4] as a possible mechanism of triggering transition of deflagration to detonation.

Modern massively parallel computers differ from each other by design substantially. Accordingly, performances of their inter-processor communications differ as well. Hence, some HPC systems and algorithms of global interprocessor communications might be more beneficial for one particular type of a parallel code than for another. In this paper we describe results of porting our Fortran-90/MPI code on SGI Altix 3700, NEC SX-8, and Cray XT4 and analyze its comparative performance for a variety of programming implementations of global communications.

In the following Section 2 we outline the governing equation and numerical algorithm to solve it. Typical results of numerical experiments with
expanding flames are illustrated in this section too. In Section 3 we describe
the structure of our computational code. Results of the benchmark runs are
presented in Section 4.

2 Mathematical Model and Numerical Algorithm

Here we study computational performance of a parallel code for numeri-
cal simulation of dynamics of three-dimensional flames using the asymptotic
model suggested in [3], where a review of other available models can be found
too.

Let us consider an expanding flame front and assume that its su-
face is close enough to a sphere and that every point on the flame sur-
face is uniquely defined by its distance $r = r(\theta, \phi, t)$ from the origin for $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$, and $t > 0$. It is convenient to represent such a flame as
a perturbation $\Phi(\theta, \phi, t)$ of a spherical surface of a reference radius $r_0(t)$, i.e. $r(\theta, \phi, t) = r_0(t) + \Phi(\theta, \phi, t)$. Denoting Fourier components of $\Phi(\theta, \phi, t)$
as $\tilde{\Phi}_k$, the Fourier image of the equation governing evolution of the three-
dimensional segments of such flames can be written as

$$
\frac{d\tilde{\Phi}_k}{dt} = \left\{ -\frac{\theta_\pi^2}{r_0(t)^2}|k|^2 + \frac{\gamma \theta_\pi}{2r_0(t)}|k| \right\} \tilde{\Phi}_k
\quad -\frac{\theta_\pi^2}{2|r_0(t)|^2} \sum_{l \in \mathbb{Z}^2} l \cdot (k - l) \tilde{\Phi}_l \tilde{\Phi}_{k-l} + \tilde{f}_k(t), \quad t > t_0 > 0,
$$

where $k = (k_1, k_2), l = (l_1, l_2)$ are pairs of integers such that $-\infty < k_i, l_i < \infty$, $i = 1, 2$, which can be denoted also as $k, l \in \mathbb{Z}^2$, $\tilde{f}_k(t)$ are the Fourier
components of the properly scaled upstream perturbations of the unburnt gas
velocity field $f(\phi, t)$, $\gamma = 1 - \rho_b/\rho_u$ is the contrast of densities $\rho_b, \rho_u$ of
the burnt and unburnt gases respectively, and initial values of $\tilde{\Phi}_k(t_0) = \tilde{\Phi}_k^{(0)}$ are
given. By construction, (1) governs dynamics of equatorial flame segments
$-\pi/(2\theta_\pi) \leq \theta \leq \pi/(2\theta_\pi), 0 \leq \phi \leq 2\pi/\phi_\pi$, where $\theta_\pi, \phi_\pi$ are integers, see [3].

For the unity Lewis number the length and time scales used in (1) are the
thermal flame front width $\delta_{th} = D_{th}/u_b$ and $\gamma^{-2}\delta_{th}/u_b$ respectively, where $D_{th}$ is the thermal diffusivity of the system and $u_b$ is the planar flame speed.
relative to the burnt gases. Choice of $r_0(t)$ in the model just introduced may be based on a variety of principles, here we use $r_0(t) = t$.

System (1) is solved numerically by neglecting the harmonics of orders higher than a finite integer number $K > 0$. Then, the nonlinearity can be represented as a circular convolution and evaluated effectively with the FFT. The structure of the two-dimensional FFT, as the tensor product of the one-dimensional ones, allows for efficient parallelization of the computational algorithm. Further details of the numerical integration algorithm can be found in [2, 3].

In spite of drastic simplifications made during evaluation of the three-dimensional asymptotic model (1), its numerical simulations are still extremely computationally intensive and computational resources available to us allowed to consider only a few cases so far. In the case presented below, the initial perturbations of the spherical flame surface were random $\Phi(\theta, \phi, t_0) = \epsilon \eta(\theta, \phi)$. Here $|\eta(\theta, \phi)| \leq 1$ is a number chosen randomly for every required combination of $\theta$ and $\phi$, $\epsilon = 10^{-3}$ and $t_0 = 200$. The explicit forcing was not applied in these examples, though the round-off errors were playing its role implicitly. Figure 1 shows evolution of half of a spherical flame in the top and of its central region in the bottom. Cells in the flame regions near the poles appear severely deformed, because of a simplified treatment of the spherical geometry in (1), and should be disregarded.

Averaged velocities of the spherical flames $<\Phi_t>$ and their power law approximations $(t - t_*)^\alpha$ are depicted in Fig. 2 as well. As time goes by, the expansion rate of the two-dimensional circular flame stabilizes to $<\Phi_t> \propto (t - t_*)^{1/4}$, i.e. to the power law predicted by the fractal analysis. The three-dimensional flames accelerate much faster than the two-dimensional ones. The power law approximation of the expansion rate on the time interval considered so far gives $\alpha \approx 0.76$, indicating good chances that the expansion rate will eventually stabilize to $<\Phi_t> \propto (t - t_*)^{1/2}$ after some transitional period as demonstrated by the experiment and predicted by fractal analysis.

Further analysis of results of numerical simulations can be found in [2, 3].

3 The structure of the computational code

The main computational array of the problem is $\tilde{\Phi}_{k_1,k_2}$, where $-K \leq k_1, k_2 \leq K$ and $K$ is a large positive integer. In order to tackle the nonlinear term in (1) as a circular convolution, the array $\tilde{\Phi}_{k_1,k_2}$ is augmented to $\Psi_{k_1,k_2}$, where
Figure 1: Evolution of half of a spherical flame (top row) and of its centrally located region (bottom row). The view in the latter sequence is limited by a cone with fixed apex angle in the origin. Here $\gamma = 0.8$ and $f(\phi, t) \equiv 0$.

Figure 2: Averaged flame front velocities and their power law approximations $(t - t_*)^\alpha$ for circular (left) and spherical (right) flames versus time $t$ (right). Here $\gamma = 0.8$ and $f(\phi, t) \equiv 0$.

$-2K \leq k_1, k_2 \leq 2K + k_0$, see e.g. [5]. The size of the augmented array is $(4K + k_0 + 1) \times (4K + k_0 + 1)$ and integer $k_0$ is selected as minimal as possible to make value of $K_\Psi = 4K + k_0 + 1$ efficient for the FFT.

Initially, the augmented array $\Psi_{k_1,k_2}$ is distributed between $N_p$ processors column-wise, so that its first $K_p = K_\Psi / N_p$ columns are stored in the first
processor, the next $K_p$ columns are in the second processor and so on. At this stage, the one-dimensional FFT can be effectively applied along the first index of the arrays $k_1 \Psi_{k_1,k_2}$ and $k_2 \Psi_{k_1,k_2}$, i.e. column-wise. In the next stage, the resulting global arrays should be transposed in order to accomplish the two-dimensional FFT by applying the one-dimensional FFT along the second index, i.e. raw-wise.

Upon completion of the two-dimensional FFT, the convolution is calculated as the element-by-element product of two FFT’ed arrays and the just describer set of operations is repeated in the backward direction. First, the one-dimensional inverse FFT is applied along the second index of the Fourier image of the convolution. Then, the global array is transposed back to its column-wise distribution and the one-dimensional inverse FFT is applied along the first index.

The overall structure of the code is illustrated in the block diagram in Fig. 3. Interprocessor communications intensive parts of the code correspond to rectangles with smoothed vertices and floating-point arithmetics intensive modules are denoted by standard rectangles. Computational resource consumption in blocks not shown in the diagram is not essential. The code was written in Fortran-90 and MPI. Vendor recommended FFT routines were used on all tested HPC systems.

The problem of transposition of data arrays distributed among a number of processors is quite common in scientific and engineering applications of HPC. A number of strategies and algorithms were suggested for various computer architectures and data structures, see e.g. [6, 7]. Here, we are considering the simplest column- and raw-wise distributions of two-dimensional arrays only and study their transpositions by straightforward MPI tools on a few popular HPC systems.

The straightforward implementation of transposition of distributed data arrays can be carried out using the **MPI_ALLTOALL** routine. Before the call to the **MPI_ALLTOALL** routine, local arrays should be reshaped, because the **MPI_ALLTOALL** routine requires the data destined for a particular processor to be stored in RAM continuously. After the call, the newly assembled local arrays should be reshaped back, now in the raw-wise manner in terms of the reference distribution of the global array, in order to apply the one-dimensional FFT along the second index. The entire procedure trebles the required memory, but RAM is usually less critical in the problem in question than the interprocessor communications efficiency. This transposition procedure is illustrated in Fig. 4 and the code itself is given in the Appendix.
Figure 3: The block-scheme of the code. Red blocks are communication and cyan ones are floating-point operations intensive.

The **MPI_GATHERV** routine can be called by every processor in order to fetch missing \((N_p - 1)K_p^2\) elements of \(\Psi_{k_1,k_2}\) and form its raw-wise repre-
Figure 4: The global data array transposition procedure. The illustration features a $6 \times 6$ array distributed over 3 processors $P_1$, $P_2$, and $P_3$.

sentation as an alternative to the use of the MPI\_ALLTOALL routine in the implementation of the global array transposition. This approach avoids reshaping of local arrays and is RAM economical. However, in our experiments all tested HPC systems performed faster with the transpositions based on the MPI\_ALLTOALL routine. As RAM is usually less critical to the problem in question than the interprocessor communications efficiency, the latter approach appears inferior to the former one on HPCs with sufficient memory resources. Accordingly, in what follows we present results for the algorithm based on the MPI\_ALLTOALL routine only.

The transposition of the global array requires in our case cross-processor transmission of $N_{\text{comm}} \propto K^2(1 - N^{-1})$ elements of $\Psi_{k_1,k_2}$ and is the most communication resource-demanding segment of the code. Combined use of the FFT routine requires $N_{fp} = \mathcal{O}(K^2\log_2 K)$ floating-point operations per time step making it the most critical arithmetic resource consumer.
Thus, the ratio of numbers of floating point to communication operations is $N_{fp}/N_{comm} = \mathcal{O}(\log_2 K_{\Psi}/(1 - N_p^{-1}))$, i.e. practically $N_{fp}/N_{comm} \approx 1$ for $N_p \gg 1$. In other words, speed of communications is as important as the speed of arithmetic operations. This is in startling contrast with explicit approximations of local PDE’s like Navier-Stokes or Maxwell systems. In the latter case explicit approximations of local derivatives would require communications just between neighbouring processors involving grid nodes from close proximities of their common boundaries only. Hence, the numbers of communication and arithmetic operations will be $N_{comm} = \mathcal{O}(K_{\Psi} N_p)$ and $N_{fp} = \mathcal{O}(K_{\Psi}^2)$, resulting in $N_{fp}/N_{comm} = \mathcal{O}(K_{\Psi}/N_p)$ and meaning that speed of interprocessor communication is not that important as speed of arithmetic operations for $N_p \ll K_{\Psi}$.

Another interprocessor communications intensive routine of our code is the symmetrization of the global solution array in order to ensure it remains real valued in physical space. Programmatically this is carried out by mapping the upper half of the global array onto the lower one in accordance with the symmetry relationship $\Psi_{-k_1,-k_2} = \overline{\Psi_{k_1,k_2}}$, see Fig. 5. The routine transmits roughly half of the array $\Psi_{k_1,k_2}$ and is called once per time step, which makes it less resource demanding than the transposition one. It is built of the non-blocking point-to-point communications subroutines MPI_ISEND and MPI_IRECV. Similarly, the numerical integration to advance the solution in time needs some floating-point arithmetics, but its resource requirements are inferior to the FFT’s.

The routine, which calculates a variety of averages of obtained numerical solution does both interprocessor communications, by using MPI_ALLREDUCE, and floating-point arithmetics. Again, its resource demands are inferior to the crucial blocks identified above. In addition, calls to this routine are not compulsory at every time step.

4 Comparative performance of the code

The Fortran-90/MPI code underwent some basic optimization during porting on a particular HPC system. Such basically optimized clones of the code were run on a set of HPCs with varying numbers of processors and solution array sizes. A few runs of the original non-optimized code have been carried out too in order to illustrate the value of adjustments to particular HPC architecture. The NEC SX-8 required the largest optimization effort, though the pay off
Figure 5: The global data array symmetrization procedure. Data from the upper-right corner are spread to the rest of the array according to the real symmetry relation $\Psi_{-k_1,-k_2} = \Psi_{k_1,k_2}$.

was the most ample too.

Figure 6: Comparison of the wall clock time $t_{N_p}$ needed to complete the task (left) and their ratios to the wall clock time for NEC SX-8 (right) versus number of processors $N_p$. Tag ini corresponds to an initial non-optimized code, its absence - to the optimized ones.

Graphs in Fig. 6 show that the code in question runs on the SX-8 on average about three times faster than on Altix and about twice faster than
on XT4. Further, they reveal that the optimized code is perfectly scalable in spite of its global all-to-all communications. Tests were carried out with $K_\Psi$ ranging from 2000 to 32000 and the graphs correspond to $K_\Psi \approx 8000$. Variations of $K_\Psi$ in the given limits does not affect behaviour of graphs in relation to each other significantly.

Figure 7: Comparison of the speed up factor $t_{N_p=4}/t_{N_p}$ versus number of processors $N_p$. Tag ini corresponds to an initial non-optimized code, its absence - to the optimized ones.

Our calculations on Altix were practically limited by 48 processors and by 32 processors on SX-8. However, it was possible to use up to 1024 processors of XT4. Corresponding graph is depicted in Fig. 7. It reveals, that scalability of the code starts to degrade from $N_p \approx 128$. However, even for $N_p = 1024$ the code manages to utilize at least 40% of the added computing power.

Profiling shows that further improvement of the code performance on all tested systems is impeded by the MPI\_ALLTOALL routine and to a lesser degree by the FFT procedures. Results of comparison of performances of our particular code on a set of HPCs should not be interpreted as the overall superiority of one of those HPCs over others.

Being computationally efficient and physically plausible, the Sivashinsky type models are not free from drawbacks. For example, they neglect certain types of low order spherical harmonics and are not valid for the entire expanding flame front, see e.g. [3]. Global geometrically correct asymptotic models were suggested as well, see e.g. [8]. In planar geometry the governing
The equation of such a model is as follows:

\[
\frac{d\mathbf{r}}{dt} = \left[-1 + \epsilon \kappa(r, t) + \frac{\gamma}{2} \left(1 + \frac{1}{\pi} \int_C \frac{(r - \xi) \cdot \mathbf{n}(r, t)}{|r - \xi|^2} dl_\xi \right)\right] \mathbf{n}(r, t). \tag{2}
\]

Here \(\epsilon\) and \(\gamma\) are physical constants, \(\kappa\) is the curvature and \(dl_\xi\) is the increment of length of contour \(C\). Other notations are explained in Fig. 8.

Figure 8: Geometry of the planar flame front \(C\) propagating outwards. \(\mathbf{n}\) is the inner unit normal.

Unlike the Sivashinsky models, the right-hand side of the latter ones cannot be represented as a tensor product of one-dimensional operators precluding use of efficient column/row-wise data structure and causing further problems in efficient parallelization. However, its singular integral in the right-hand side can be treated with the fast multipole techniques \[9\] reducing the number of required floating point operations per time step to roughly \(N_{fp} = \mathcal{O}(K^2)\). The number of required communications per time step will be in the range \(\mathcal{O}(K^2) < N_{comm} < \mathcal{O}(N_pK^2)\), meaning that the efficiency of computations with this model will be defined by the quality of programming and acceptable compromise with accuracy.

On the other hand, explicit economical discretization of the 3-D Navier-Stokes system would lead to \(N_{fp} = \mathcal{O}(K^3)\), and approximately the same
number of communications. It should be noticed however, that approximation of the Navier-Stokes system in the radial direction would need much larger number of grid nodes than in the azimuthal ones, $K$, in order to resolve the structure of the flame front. Furthermore, the Navier-Stokes approach would need to operate with a large set of physical parameters, e.g. concentrations of reacting chemical species. Thus, it appears that for practical values of $K$, arithmetic and communication demands of the Navier-Stokes models will be greater than of model [8]. Although, complexity of approximation of the singular integral and the asymptotic nature of model [8] may annul the benefit of reduction of the problem dimension by one.

5 Conclusions

Global data array transposition is the most resource consuming operation in simulations in question. Developed MPI code based on a Sivashinsky type model and MPI_ALLTOALL routine for transposition of column-wise distributed data arrays is perfectly scalable for up to a hundred of processors. On Cray XT4 increase of $N_p$ from 128 to 1024 utilizes at least 40% of added computational power. Performance of the NEC SX-8 both as a massively parallel system and as a “number cruncher” is superior to other tested systems. Achieving reasonable code efficiency requires intensive optimization on all considered systems.

Extrapolation of the Cray XT4 and NEC SX-8 performance shows that with their help reaching the stabilized acceleration regime of the expanding three-dimensional spherical flame numerically is feasible. Studies of the auto-transition of such flames to detonation on this computer are realistic as well. Prospects of use of massively parallel systems for more sophisticated asymptotic models of flame dynamics are less encouraging, but not hopeless.

Comparison of performances of computers was carried out on a particular code only and should not be interpreted as the overall superiority of one HPC system over another.

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Appendix. The Fortran 90/MPI distributed array transposition routine

```fortran
MODULE sphe_d2_mpi_mach
  INTEGER, PARAMETER :: ikd=KIND(1) ! main integers
  INTEGER, PARAMETER :: rkd=SELECTED_REAL_KIND(P=15) ! main reals
  INTEGER, PARAMETER :: ikd0=KIND(1) ! MPI integers
END MODULE sphe_d2_mpi_mach

SUBROUTINE Transp2(u,v,nproc,Kex,nconv,nconv_mpi,ut,vt)
  ! Row-to-column transposition of [-Kex:nconv-Kex-1]x[-Kex:nconv-Kex-1]
  ! distributed in chunks of [-Kex:nconv-Kex-1]x[1:nconv_mpi] arrays
  ! over nproc processors
  !
  ! u,v - initial and transposed arrays correspondingly
  ! nproc - number of processors
  ! Kex=2*K
  ! nconv=4*K+k0+1
  ! nconv_mpi=nconv/nproc
  ! ut,vt - internal work arrays
  !
  USE sphe_d2_mpi_mach
  USE MPI
  IMPLICIT NONE
  INTEGER(KIND=ikd0) :: ier_mpi
  INTEGER(KIND=ikd) :: j,l,nproc,Kex,nconv,nconv_mpi
  REAL(KIND=rkd) :: u(-Kex:nconv-Kex-1,1:nconv_mpi)
  REAL(KIND=rkd) :: v(-Kex:nconv-Kex-1,1:nconv_mpi)
  REAL(KIND=rkd) :: ut(1:nconv_mpi*nconv_mpi,1:nproc)
  REAL(KIND=rkd) :: vt(1:nconv_mpi*nconv_mpi,1:nproc)

  ! Executables ----------------------------------------------------
  IF(nproc==1)THEN
    DO j=-Kex,nconv-Kex-1
      v(:,j+Kex+1)=u(j,:)
    END DO
  END IF
END SUBROUTINE Transp2
```
ELSE
  DO l=1,nproc
    DO j=1,nconv_mpi
      ut((j-1)*nconv_mpi+1:j*nconv_mpi,l) &
      & =u((l-1)*nconv_mpi-Kex:l*nconv_mpi-Kex-1,j)
    END DO
  END DO
  CALL MPI_ALLTOALL(ut,nconv_mpi*nconv_mpi,MPI_DOUBLE_PRECISION, &
                    vt,nconv_mpi*nconv_mpi,MPI_DOUBLE_PRECISION, &
                    MPI_COMM_WORLD,ier_mpi)
  DO j=1,nconv_mpi
    DO l=1,nproc
      v((l-1)*nconv_mpi-Kex:l*nconv_mpi-Kex-1,j) &
      & =vt(j:(nconv_mpi-1)*nconv_mpi+j:nconv_mpi,l)
    END DO
  END DO
END IF
RETURN
END SUBROUTINE Transp2