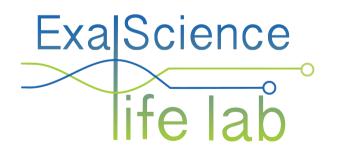
Parallel Matrix Factorization





Tom Vander Aa and Tom Ashby

EuroMPI Tutorial on Machine Learning at Scale



















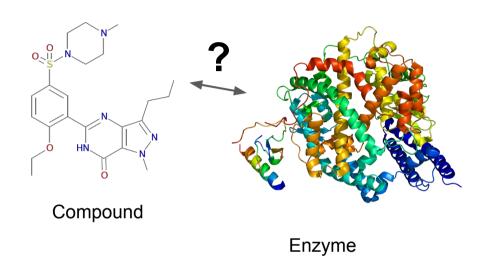
Overview

- Introduction
 - Compound Activity Prediction
 - BPMF
- Single node
 - Shared memory parallelism
 - Load balancing
- Distributed
 - Communication-computation overlap
 - Results

Compound Activity Prediction

Predict

- compound activity on
- protein target
- aka chemogenomics



Similar to

- Netflix: users rating movies
- Amazon: users rating books





Chemogenomics: Background

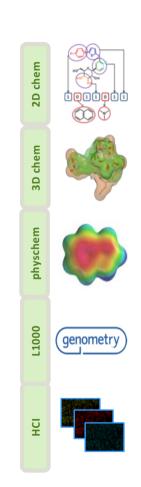
~1% can be filled up with experimental dose response data

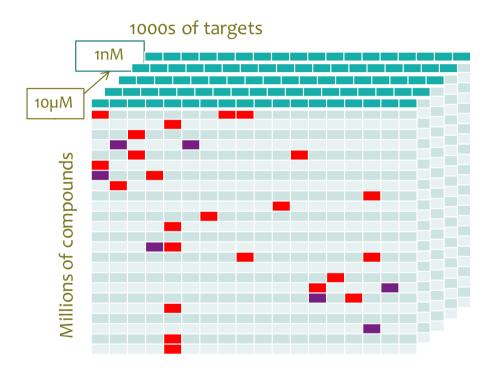




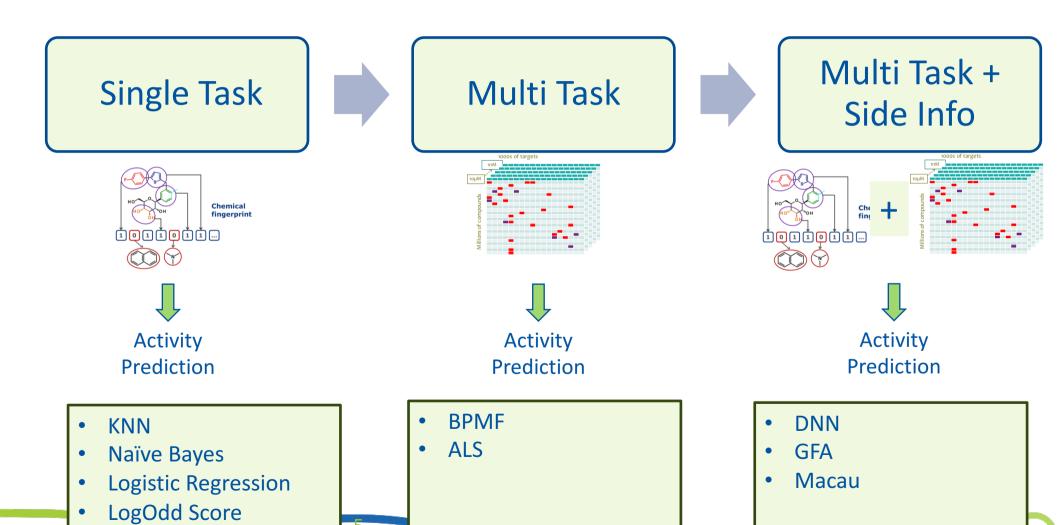


Quarterly updated





Several Methods Developed



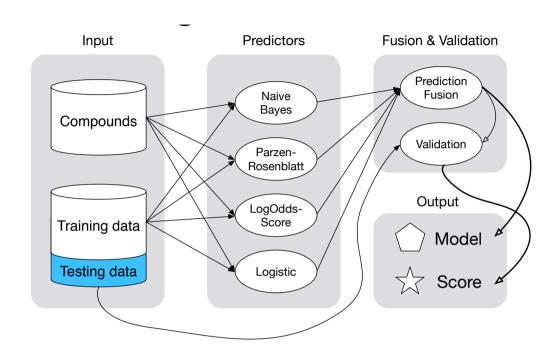
Single Task Learning with Spark

Dimensions:

- Cross-Fold
- Parameter Search
- Activity Levels
- Compound

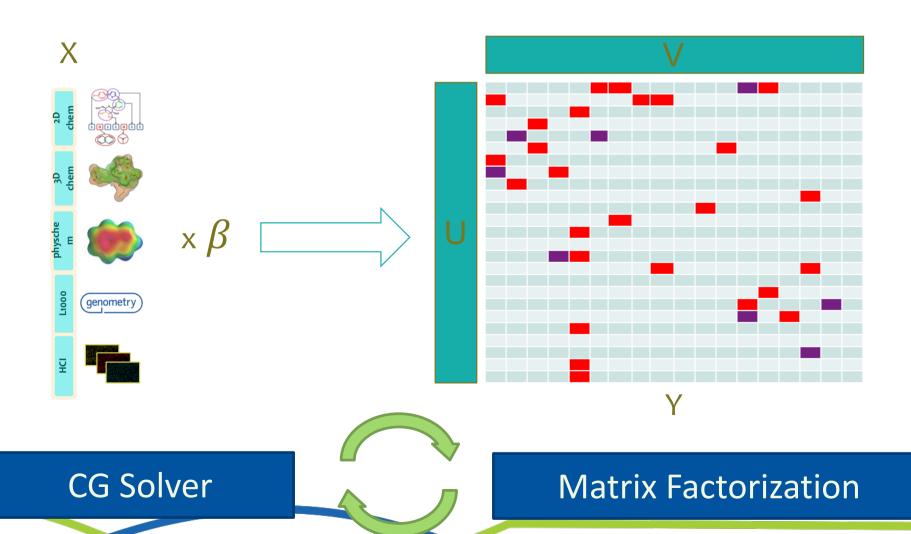


= Embarrassingly Parallel



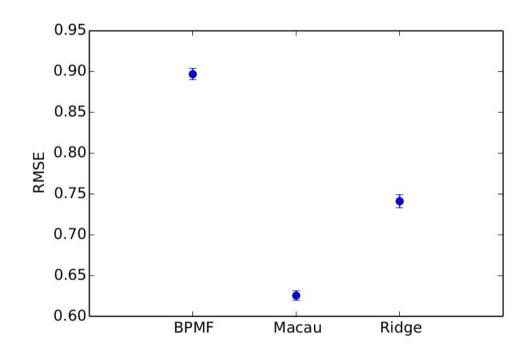


MACAU: Multi-Task Learning with Side Info

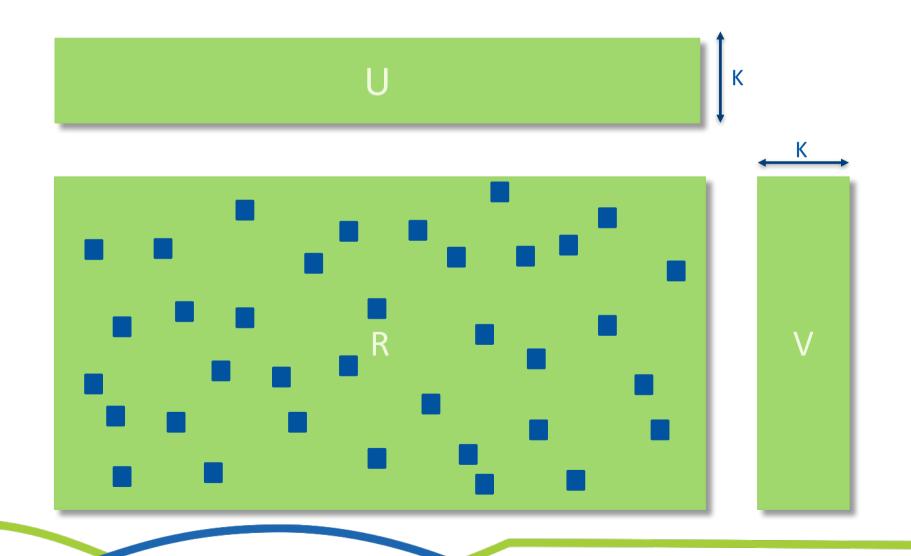


Added Value of Compound Features

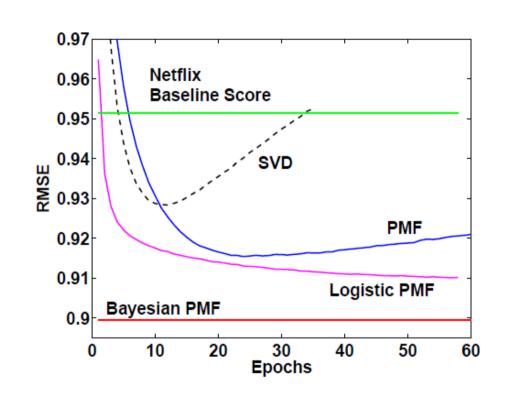
- Version: ChEMBL v19
 - o 346 proteins
 - o 15,073 compounds
 - o 59,280 IC50 measurements
- 105k dimensional ECFP features
- Use 20% as test set
- 10 repeats
- D = 30 (#latent dimensions)

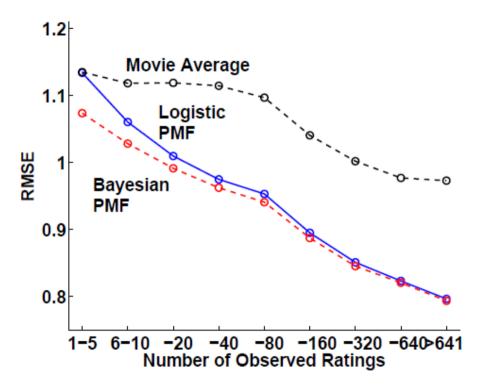


BPMF := Low-rank Matrix Factorization



BPMF seems to predict well





Bayesian: all possible models

Priors and HyperPriors: Users are Gaussian distributed

Gibbs sampling

BPMP: simple, promising but slow

BPMF is simple

- 25 lines of Julia code
- 35 lines of C++ code

BPMF predicts well

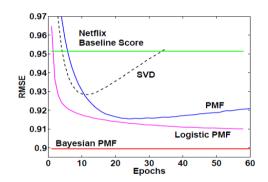
- by using Bayesian approach
- by using compound fingerprints in Macau

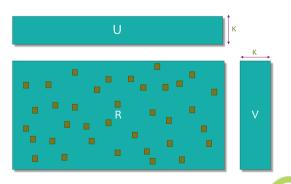
BPMF is slow

- Sampling based
- Julia prototype: 15 days / run









Baseline BPMF is simple

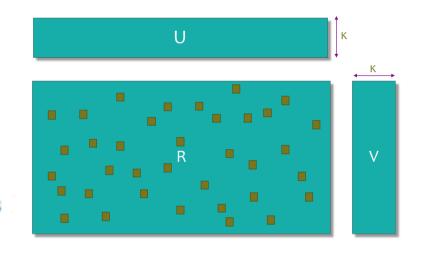
For t=1,...,T

Sample the hyperparameters

$$\Theta_U^t \sim p(\Theta_U|U^t, \Theta_0)$$

 $\Theta_V^t \sim p(\Theta_V|V^t, \Theta_0)$

- For each i = 1, ..., N sample user features $U_i^{t+1} \sim p(U_i|R, V^t, \Theta_U^t)$
- For each i = 1, ..., M sample movie features $V_i^{t+1} \sim p(V_i|R, U^{t+1}, \Theta_V^t)$



Typical Input Data

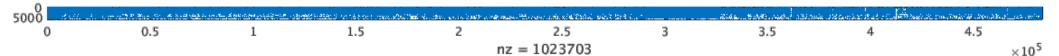
Parameters

- Number of latent features: 100
- Number of sampling iterations: 1000

Industrial Data

- 1.7M compounds
- 2350 targets
- 36.7M entries (0.8%)



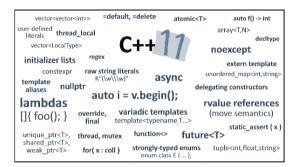


Single Node Implementation

Operations

- Matrix/Vector operations
- Matrix inversion / Cholesky
- Random numbers
- Typically on: KxK matrices
 - K: number of latent features
 - Typical K == 100

- Choice of tools
 - C++
 - TBB/OpenMP
 - Eigen 3.3







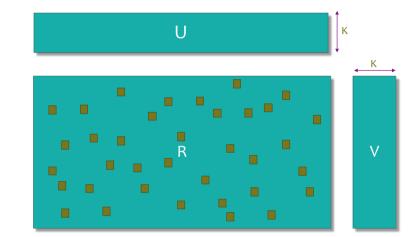
Single Core Optimizations

- Algorithmic
 - Full Inverse vs Cholesky vs Cholesky + rank update
- Eigen
 - Optimize expression templates
 - Annotate aliasing in matrix operations

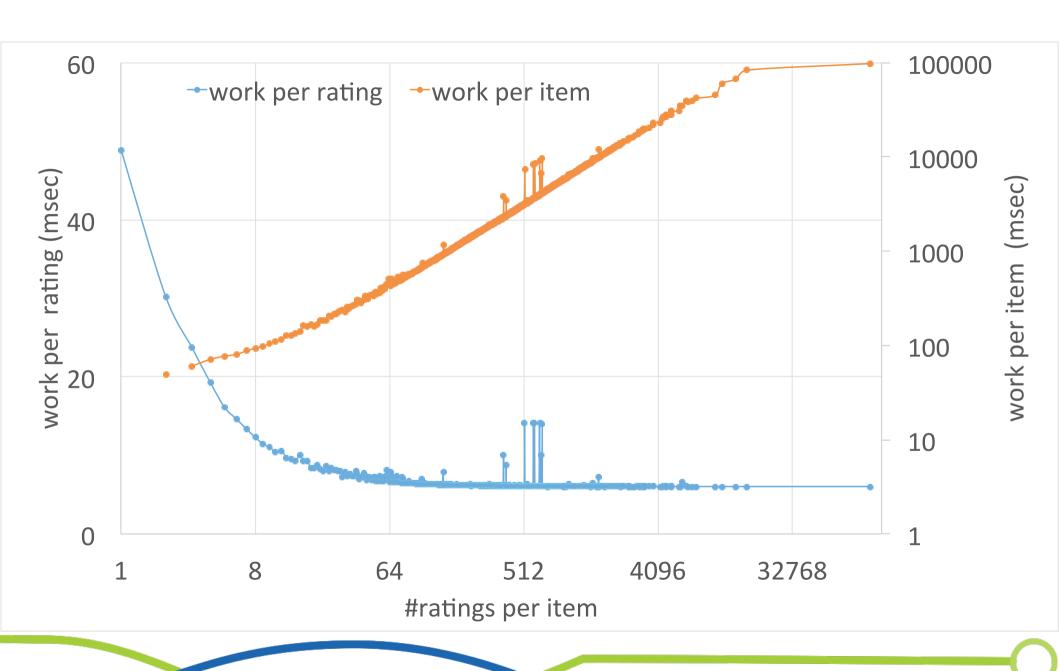
- Compute in one pass over U
 - Norm, Average, Covariance, Updated U

Single Node Parallelization

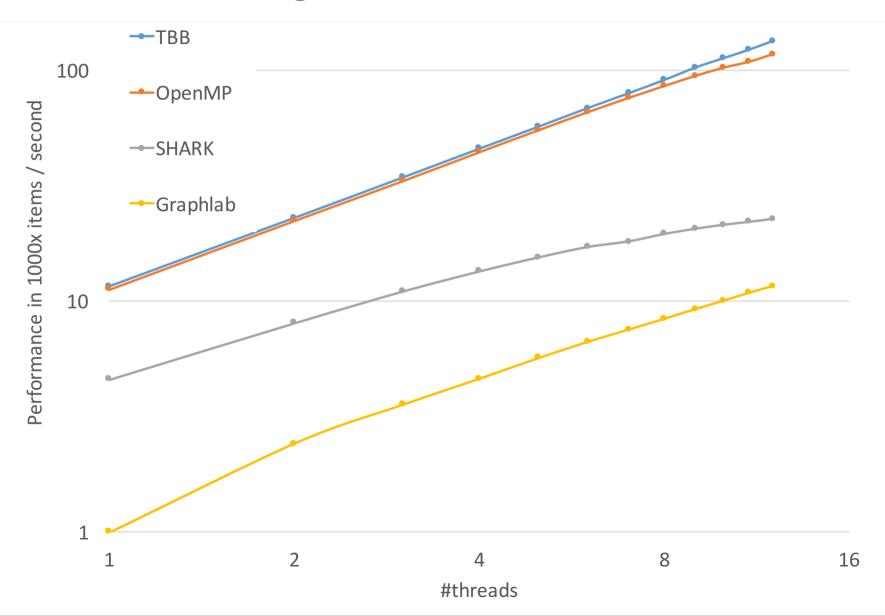
- Seems easy to parallelize
 - Across users/movies
 - Inside a user/movie
 - Compute Precision matrix
- Shared memory parallelism
 - Memory bandwidth limited
 - Optimize rank R matrix for locality



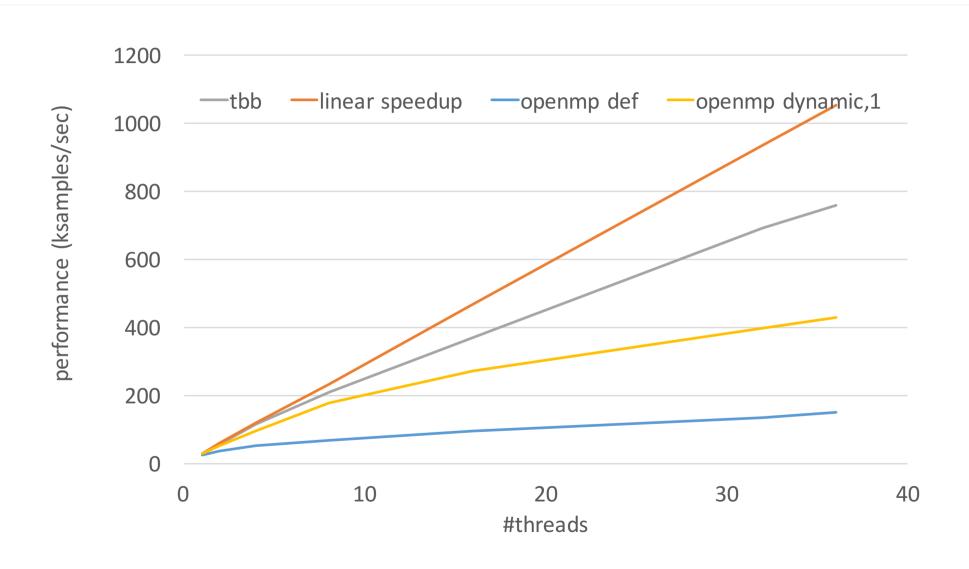
- Load Balancing
 - Load depends on #items, and #nnz
 - Use TBB nested parallelism across + inside items



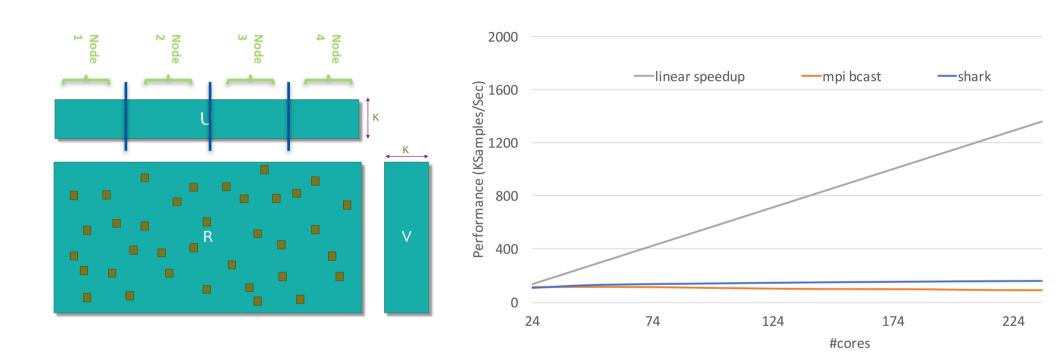
Single Node Performance



Single Node Performance



Synchronous Distributed BPMF



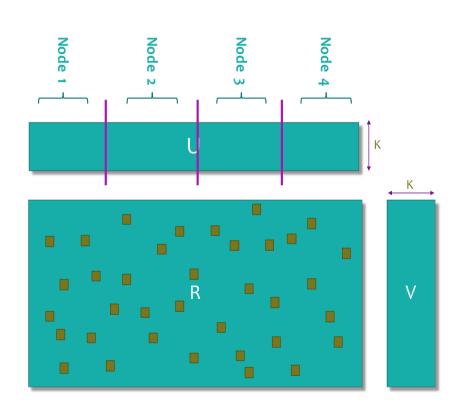
Only 2x improvement with 20x more cores
We need asynchronous communication

EXA2CT Slides

Asynchronous Distributed BPMF

- Split both U/V, optimizing:
 - Load balance (# rows, #nnz)
 - Communication
 - → Both are determined by R

- Basic Pattern GASPI
 - Compute a column of U/V
 - Send to needed nodes



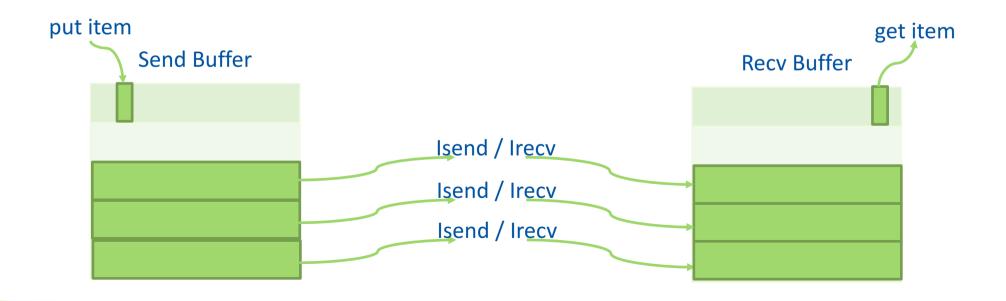
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 1307 1689 | | | | | | | | | | 1517 1669 | | 644 1706 |
|----------------------------------|------------------|--------------|------------------------|------|------------------------|------|--------------|----------------------|--------------------|------|------------------|------------------------|--------------|--------------------|--------------------|--------------|--------------|--------------------|--------------------|------------------|--------------|--------------|------------------------|--------------|--------------|--------------------|--------------------|----------------------|--------------------|--------------------|--------------------|------------------------|--------------|------------------------|--------------|--------------------|----------------------|--------------|------------------|------------------------|--------------|------------------------|--------|----------------------|
| 1425 0 1683 1472 1492 0 | | | 1526 1552 | | 1546 148 1595 1517 | 1424 | 1510 | 1534 142 | 5 1499 | 1530 | 1435 1 | 468 1569 | 14/1 | 1392 15 | 06 1535 nr 1574 | 1518 | 1493 | 1450 15 | 14 1500 74 1516 | | | | 1502 1504 1520 1500 | 1581 | | 1512 15 1554 14 | 14 1565 | 1491 142 | 3 1433 | 1484 14 | 85 1538 77 1400 | 1495 1590 1452 1595 | | 516 1474 519 1535 | 1535 | 1565 15 | 590 1497 | 1552 | 1632 | 1556 1478 | 1553 1550 | 1553 1589 | 1661 1 | 545 1679 |
| 1315 1592 1529 | | | 1502 1017 | | 1652 151 | 1581 | 1573 | 1555 154 | 10 1460 16 1434 | 1600 | 1900 1 | 440 1302 1655 1655 | 1345 | 1319 15 | 90 1504 89 1500 | 1559 | 1505 | 1583 15 | | | | | 1628 1558 | 1657 | | 1428 13 | 3 1606 | 1615 159 | 15 1372 | 1410 15 | 11 1492 | 1352 1591 | | | 1525 | 1509 16 | 665 161R | 1546 | 1564 1 | 1573 1585 | 1641 | 1498 1697 | 1630 1 | 520 1076 651 1710 |
| 1401 1461 1490 | | | 1654 1646 | | 1633 1476 | 1478 | 1533 | 1515 149 | 99 1415 | 1550 | 1389 1 | 1421 1527 | 1439 | 1365 15 | | 1475 | | 1474 15 | | | | | 1511 1519 | | | 1460 14 | | 1530 152 | | 1399 15 | 40 1605 | 1484 1597 | | 597 1416 | | 1578 16 | 638 1580 | 1558 | 1558 | 1574 1454 | 1543 | 1481 1605 | 1676 | 611 1626 |
| 1418 1454 1488 | 8 1530 | 1467 | 0 1732 | 1519 | 1684 150 | 1496 | 1577 | 1556 146 | 58 1451 | 1547 | 1446 1 | A27 1583 | 1479 | 1427 15 | 59 1578 | 1487 | 1529 | 1447 14 | 93 1474 | 1478 | 1527 | 1619 | 1497 1507 | 1560 | 1613 | 1515 14 | 1607 | 1522 146 | 3 1448 | 1515 14 | 75 1537 | 1473 1630 | 1549 | 513 1484 | 1551 | 1586 16 | 639 1563 | 1549 | 1616 | 1563 1486 | 1622 | 1518 1600 | 1653 1 | 566 1654 |
| 1485 1457 1493 | 2 1541 | 1474 | 1473 0 | | 1688 1568 | 1511 | 1512 | 1566 142 | 1492 | 1447 | 1479 1 | 481 1542 | 1450 | 1468 14 | 71 1595 | 1516 | 1499 | 1478 15 | 15 1494 | 4 1502 | 1503 | 1594 | 1499 1629 | 1546 | 1593 | 1514 15 | 1541 | 1503 143 | 19 1487 | 1424 14 | 87 1542 | 1512 1532 | | 593 1484 | 1553 | 1541 15 | 584 1581 | 1517 | 1596 ! | 1636 1490 | 1531 | 1565 1582 | 1666 1 | 615 1638 |
| 1308 1511 1494 | 4 1428 | | 1528 1626 | | 1781 1523 | | 1653 | 1615 163 | 31 1341 | 1689 | 1273 1 | 376 1667 | 1325 | 1280 16 | 07 1471 | 1536 | | 1600 15 | 69 1453 | | 1586 | 1588 | 1597 1465 | | | 1451 12 | | 1622 158 | | 1413 15 | | 1318 1698 | | 635 1410 | | 1583 17 | 732 1625 | 1533 | 1528 | 1553 1523 | 1673 | 1491 1644 | 1643 1 | 628 1737 |
| 1445 1482 1494 1321 1480 1493 | 4 1542 3 1502 | | 1516 1515 1484 1577 | | 101 | | | 1567 149 1591 157 | | 1466 | 1458 1 | 1483 1566 1440 1554 | 1469 | 1421 15 | 10 1540 cc 1520 | 1527 | | 1503 15 | | | 1546 | | 1556 1527 1529 1532 | | | 1519 15 1434 13 | 23 1585 90 1603 | 1523 142 1596 161 | | | | | | 511 1490 625 1457 | | 1563 15 | 589 1523 | 1523 | 1572 1 | 1591 1506 | 1586 | 1531 1581 | 1626 1 | 553 1679 COD 1714 |
| 1457 1492 1466 | | | | | 1524 148 | | | 1650 150 | | 1541 | 1469 1 | 1436 1600 | 1493 | 149) 14 | 00 1330 96 1607 | 1491 | | | | | | | | | | | | 1499 135 | | | | | | | | 1619 16 | 667 1518 | 1604 | 1640 | 15% 1.059 | 1583 | 1614 1555 | 1627 1 | 029 1714 544 1646 |
| 1420 1447 1416 | | | 1478 1478 | | 1540 144 | 1435 | 0 | 1665 155 | | 1480 | | 1519 1571 | 1451 | 1459 14 | R2 1561 | | | 1471 14 | | | | | 1492 1550 | | | | | 1534 142 | | 1484 14 | | | 1580 | | | | 605 1551 | 1552 | 1617 | 1609 1546 | 1554 | 1556 1594 | 1585 1 | 578 1634 |
| 1407 1489 1527 | 7 1481 | 1492 | 1518 1467 | 1429 | 1562 1474 | 1456 | 1480 | 0 161 | 18 1568 | 1479 | 1503 1 | 1519 1627 | 1458 | 1469 15 | 46 1510 | 1549 | 1524 | 1519 15 | 28 1498 | 3 1465 | 1494 | 1579 | 1547 1535 | 1547 | 1600 | 1482 15 | 22 1508 | 1574 147 | 2 1480 | 1425 15 | 17 1548 | 1493 1568 | 1569 | 601 1495 | 1519 | 1554 16 | 630 1588 | 1517 | 1522 | 1588 1576 | 1583 | 1543 1594 | 1620 1 | 569 1632 |
| 1454 1436 1495 | 5 1578 | 1486 | 1455 1465 | 1496 | 1519 144 | 1366 | 1460 | 1492 | 0 1672 | 1439 | 1571 1 | 533 1602 | 1535 | 1492 14 | 83 1607 | 1475 | 1534 | 1437 14 | 89 1512 | 2 1500 | 1536 | 1608 | 1500 1545 | 1492 | 1593 | 1526 15 | 56 1574 | 1457 135 | 7 1520 | 1494 14 | 54 1475 | 1532 1548 | 1549 | 511 1491 | 1573 | 1565 19 | 596 1539 | 1548 | 1599 | 1554 1494 | 1521 | 1584 1548 | 1626 1 | 551 1647 |
| 1362 1514 1545 | 9 1503 | 1490 | 1524 1545 | 1352 | 1566 144 | 1478 | 1534 | 1544 153 | 31 0 | 1581 | 1545 1 | 505 1644 | 1418 | 1340 16 | 02 1550 | 1544 | 1500 | 1567 15 | 38 1467 | 7 1508 | 1558 | 1585 | 1601 1538 | 1577 | 1621 | 1466 13 | 95 1570 | 1594 153 | | 1460 15 | 55 1604 | 1404 1610 | | 623 1430 | 1551 | 1574 16 | 637 1602 | 1543 | 1602 ! | 1608 1515 | 1595 | 1516 1659 | 1630 1 | 606 1702 |
| 554 581 559 1332 1521 1501 | 9 589 | | 5/2 586 1458 1578 | 1212 | 1570 1399 | 1506 | 1000 | 568 56 1539 152 | | 16(1 | 0 1 | 556 570 1522 1749 | 1/50 | 1275 15 | /5 5/4 07 150/ | 1524 | 1/02 | 1520 15 | 80 561 80 1494 | 1 561 | 1566 | 1502 | 5// 565 156/ 1577 | 5/5 1500 | 593 1622 | | 58 575 28 1630 | 572 60 | 12 564 30 1384 | | 61 592 no 1566 | 567 594 1406 1677 | | 594 552 584 1457 | 1517 | 569 6 1592 16 | 668 1623 | 1563 | 1604 | 569 572 1576 1471 | 15/0 | 585 581 1510 1636 | 1656 1 | 582 590 534 1730 |
| 1352 1321 1301 | | | 1519 1568 | | 1578 1412 | 1473 | | 1557 147 | | | 1386 | 0 1793 | | 1365 16 | | 1500 | | 1507 15 | | | 1565 | | 1585 1488 | | | | | 1549 154 | | 1441 14 | | 1449 1657 | | | | | 653 1562 | 1589 | 1570 | 1577 1456 | 1575 | 1538 1614 | 1687 | 566 1716 |
| 1483 1449 1495 | | 1461 | 1490 1521 | | 1505 148 | 1383 | 1445 | 1462 142 | 27 1529 | 1458 | 1485 1 | 502 0 | | | 48 1638 | | 1530 | | | | 1572 | | | | | | | | | | | 1552 1522 | | 481 1494 | | 1580 15 | | 1600 | 1629 | 1577 1497 | 1568 | 1588 1575 | 1644 | 503 1652 |
| 1313 1484 1501 | | 1486 | 1511 1574 | 1320 | 1619 1419 | 1532 | 1549 | 1531 154 | 19 1374 | 1590 | | 1427 1618 | | 1446 17 | | | | 1582 16 | 05 1498 | 3 1484 | 1542 | | 1593 1563 | | | 1475 14 | | 1608 159 | | 1456 15 | | | | | | 1592 17 | 706 1659 | 1528 | 1564 1 | 1600 1529 | 1614 | 1483 1663 | 1677 1 | 676 1736 |
| 1246 1520 1547 | 7 1421 | 1519 | 1528 1590 | 1283 | 1631 1411 | 1606 | 1599 | 1555 158 | 86 1309 | 1703 | 1265 1 | 1325 1675 | 1298 | 0 17 | 89 1674 | | | 1623 16 | 07 1499 | 2 1529 | 1680 | 1648 | 1617 1574 | 1617 | 1687 | 1404 12 | 27 1660 | 1646 165 | | 1385 16 | | | 1483 | 671 1416 | 1465 | 1581 17 | 700 1643 | 1486 | 1619 | 1591 1513 | 1673 | 1505 1693 | 1642 1 | 635 1788 |
| 1453 1440 1496 1392 1516 1463 | 6 1623 3 1466 | 1519 1471 | 1487 1474 1542 1517 | 1449 | 1513 1477 1559 1411 | 1417 | 1468 | 1520 141 | 1492 | 1472 | 1486 1 | 1453 1505 | 1531 | 1483 | 0 1727 | 1632 | 1585 | 1540 15 | 45 1526 | 1560 | 1522 | 15/2 | 14/5 1550 | 1583 | 1550 | 1502 15 | 46 1556 16 1604 | 1506 140 | | 1468 14 | 80 1529 40 1567 | 1555 1552 | | 482 1512 | 1581 | 1593 16 | 600 1545 | 1542 | 1642 | 1623 1480 | 1542 1644 | 1595 1618 | 1626 1 | 545 1662 cnc 1ccn |
| 1392 1516 1463 1399 1497 1546 | | | 1542 1517 1469 1545 | 1476 | 1555 1411 | 1320 | 1539 | 1514 130 | 1 1447 | 1550 | 1381 1 | 388 1572 | | | 42 <u> </u> | 1009 | 1682 | 1530 15 | 1/ 149) 89 154) | 1 1543 2 1467 | 1510 | 1609 | 1559 1468 | 1544 | 1620 | 1541 14 | 16 1604 53 1560 | 1631 153 1503 144 | | | 49 1567 88 1522 | 1435 1597 1499 1594 | | 585 1452 547 1489 | 1501 | 1581 II 1594 14 | 000 1016 645 1548 | 1585 | 1564 | 1541 1444 | 1574 | 1560 1540 | 1666 1 | 568 1690 |
| 1382 1512 1504 | | | 1502 1512 | 1364 | 1581 144 | 1476 | 1421 | 1518 148 | 8 1411 | 1552 | 1366 1 | 1429 1576 | | | | 1508 | | 1675 16 | | | 1579 | | 1531 1577 | | | 1466 14 | | 1561 152 | | | | | 1544 | | | 1506 16 | 680 1588 | 1505 | 1558 | 1608 1512 | 1570 | 1486 1605 | 1608 1 | 510 1544 511 1544 |
| 1475 1430 1495 | 3 1599 | 1506 | 1431 1551 | 1480 | 1511 145 | 1352 | 1479 | 1479 135 | 58 1477 | 1468 | 1455 1 | A59 1583 | 1529 | 1463 14 | 51 1568 | 1417 | 1530 | 0 16 | 96 1619 | 5 1574 | 1596 | 1608 | 1524 1484 | 1517 | 1580 | 1542 15 | 57 1610 | 1509 139 | 1475 | 1515 14 | 73 1468 | 1549 1581 | 1514 | A61 1523 | 1551 | 1650 16 | 618 1518 | 1507 | 1627 | 1593 1463 | 1593 | 1597 1559 | 1655 1 | 551 1664 |
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| 1384 1466 1485 | 5 1477 | | 1480 1541 | 1398 | 1597 1485 | 1520 | 1553 | 1503 148 | 32 1382 | 1539 | 1387 1 | 444 1622 | 1345 | 1385 15 | 48 1564 | 1528 | | 1491 15 | - | 1660 | | | 1626 1594 | | | 1460 14 | 16 1659 | 1595 156 | 9 1412 | 1440 15 | | 1413 1598 | | 655 1444 | | 1547 16 | 653 1645 | 1504 | 1605 ! | 1599 1576 | 1582 | 1516 1645 | 1679 1 | 689 1707 |
| 1373 1486 1563 1410 1513 1503 | 3 1509 | 1519 | 1505 1607 1464 1400 | 1373 | 1585 148 | 1443 | 1558 | 1501 149 | H 1366 | 1607 | 1391 1 | 586 1641 1622 1000 | 1435 | 1875 15 | 64 1502 no 1400 | 1483 | 1540 | 1493 15 | 19 1486 44 1417 | 7 1450 | 1715 | 1736 1756 | 1654 1502 1696 1564 | _ | | 1540 14 1509 14 | 22 1625 | 1628 147 1533 147 | 3 1390 10 1467 | 1469 15 | 25 1537 40 1642 | 1429 1672 1434 1609 | | .613 1435 .640 1423 | | 1594 16 | 651 1541 | 1550 | 1568 1 | 1574 1461 | 1649 | 1562 1610 | 1629 1 | 564 1677 cac acac |
| 1410 1515 1500 | 0 1547 | 1503 | 1404 1477 | 1348 | 1430 1431 | 1455 | 1451 | 1900 193 | 77 1404 75 1464 | 1533 | 1422 1 | 1433 1399 1488 1574 | 1424 | 1429 15 | 12 1463 17 1463 | 1523 | 1492 | 1492 15 | | _ | 1542 | | 1720 1595 | | | 1675 15 | 08 1619 | 1579 147 | 19 1407 14 1511 | 1505 15 | 49 1043 19 1581 | 1500 1583 | | | | 1558 16 | 649 1585 | 1574 | 1573 | 1557 1543 | 1555 | 1534 1677 | 1628 1 | 940 1030 609 1687 |
| 1422 1435 1514 | | | 1468 1511 | 1417 | 1571 141 | 1428 | 1478 | 1551 143 | 37 1454 | 1504 | | 1450 1531 | | 1415 14 | 66 1612 | 1505 | 1520 | | 89 1500 | | | 1568 | | | 1690 | | 79 1677 | 1523 144 | 3 1497 | 1533 15 | | 1515 1607 | | 517 1522 | | | 592 1561 | 1556 | 1657 | 1591 1480 | 1559 | 1571 1630 | 1662 | 595 1669 |
| 1438 1516 1538 | 8 1609 | 1560 | 1531 1610 | 1377 | 1601 148 | 1437 | 1541 | 1584 149 | 33 1453 | 1615 | 1367 1 | 1432 1629 | 1467 | 1436 15 | 27 1539 | 1460 | 1512 | 1458 15 | 27 1535 | 5 1439 | 1535 | 1570 | 1552 0 | 1662 | | 1592 14 | | | 4 1491 | 1564 14 | 86 1519 | 1503 1638 | 1563 | 501 1507 | 1566 | 1618 16 | 666 1564 | 1613 | 1595 | 1545 1463 | 1658 | 1621 1628 | 1699 1 | 532 1684 |
| 1135 1151 1165 | | | 1111 1142 | 1107 | 1137 107 | 1071 | 1153 | 1122 106 | 57 1113 | 1093 | 1100 1 | 1128 1146 | | 1108 11 | 11 1168 | 1081 | 1144 | 1066 11 | 01 1094 | | | | 1116 1145 | | | | | 1104 106 | | 1161 11 | | 1149 1143 | | | | 1193 12 | 255 1199 | 1152 | 1187 | 1205 1119 | 1165 | 1286 1178 | 1275 1 | 205 1270 |
| 1133 1184 1183 1312 1517 1508 | 2 1236 8 1430 | 1240 | 1228 1244 1514 1550 | 1126 | 1225 114 | 1147 | 1177 | 1211 114 | 13 1166 17 1359 | 1272 | 1119 1 | 1174 1260 1383 1672 | | 1192 11 1277 16 | 95 1231 05 1508 | 1223 1504 | 1194 | 1195 11 1608 15 | 81 1238 54 1460 | | 1256 | | 1220 1205 1563 1546 | | 1647 | | | 1309 113 1733 157 | | 1228 12 | | 1185 1273 1373 1647 | | 212 1222 655 1431 | | 1259 13 | 309 1251 | 1270 | 1278 | 1256 1188 | 1275 | 1313 1302 | 1261 1 | 249 1375 |
| 963 1220 1193 | | | 1162 1257 | | 13/1 141: | 1214 | 1350 | 1900 131 | 17 931 | 1351 | 910 1 | 1002 1297 | | | 77 1161 | | | 1744 11 | 34 140. R1 1107 | | 1779 | | | | | | | 1236 127 | | 1372 15 1107 11 | | | | 000 1401 267 1061 | 1147 | 1224 14 | 411 1791 | 1150 | 1207 1 | 1175 1176 | 1273 | 1129 1283 | 1314 1 | 006 1067 254 1441 |
| 1457 1466 1465 | 5 1522 | 1464 | 1495 1494 | 1421 | 1568 1526 | 1422 | 1476 | 1449 146 | 3 1453 | 1512 | 1462 1 | .468 1541 | 1485 | 1436 14 | 65 1525 | 1478 | 1491 | 1481 15 | 10 1477 | 7 1448 | 1491 | 1495 | 1555 1520 | 1551 | | 1498 14 | 34 0 | 1725 141 | 3 1597 | 1431 15 | BS 1634 | 1530 1644 | 1589 | 585 1491 | 1566 | 1570 16 | 631 1605 | 1563 | 1624 | 1594 1523 | 1603 | 1590 1606 | 1687 1 | 612 1638 |
| 1464 1460 1485 | 5 1566 | 1518 | 1455 1520 | 1468 | 1502 147 | 1404 | 1477 | 1531 142 | 28 1477 | 1432 | 1465 1 | 1466 1525 | 1508 | 1488 14 | 30 1573 | 1508 | 1517 | 1451 14 | 67 1467 | 7 1476 | 1518 | 1554 | 1492 1543 | 1540 | 1595 | 1521 15 | 13 1538 | 0 136 | 6 1589 | 1538 15 | 80 1542 | 1583 1629 | 1596 | 534 1575 | 1596 | 1576 15 | 583 1557 | 1588 | 1629 | 1566 1522 | 1577 | 1547 1605 | 1636 1 | 519 1641 |
| 1521 1440 1520 | | | 1464 1516 | | 1505 1457 | 1345 | | 1521 134 | | 1459 | 1452 1 | 1446 1513 | | 1438 14 | | | | | 86 1521 | | | 1518 | 1469 1503 | | | | | 1442 | | 1507 13 | | _ | | A14 1493 | | 1570 19 | 581 1449 | 1546 | 1604 | 1552 1442 | 1525 | 1614 1527 | 1783 1 | 495 1641 |
| 1236 1553 1555 | | | 1540 1626 | 1303 | 1659 1424 | 1572 | 1583 | 1568 157 | 76 1285 | 1686 | 1298 1 | 365 1652 | | 1182 16 | | | | 1562 15 | | | | | 1591 1546 | 22.00 | | | | 1615 165 | | 1381 17 | | | | | | 1633 17 | 732 1685 | 1558 | 1602 | 1596 1534 | 1658 | 1483 1686 | 1678 1 | 670 1720 |
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| 1475 1467 1504 | | | 1496 1510 | 1445 | 1495 146 | 1359 | 1518 | 1536 139 | 94 1504 | 1481 | 1467 1 | 1454 1533 | 1509 | 1443 14 | 58 1547 | | | 1442 14 | | | | | 1486 1489 | | | 1568 15 | | 1484 137 | | 1543 14 | | 1655 1710 | | | | 1623 19 | 581 1525 | 1610 | 1619 | 1587 1489 | 1596 | 1640 1602 | 1631 | 508 1633 |
| 1186 1549 1511 | 1 1412 | 1485 | 1512 1632 | 1225 | 1653 140 | 1575 | 1572 | 1551 160 | 00 1293 | 1705 | 1263 1 | 345 1708 | 1248 | 1150 16 | 37 1546 | 1514 | 1497 | 1654 15 | 69 1416 | 5 1439 | 1559 | 1643 | 1579 1532 | 1630 | 1670 | 1418 12 | 72 1664 | 1628 167 | 4 1228 | 1396 15 | 16 1646 | 0 1860 | 1508 | .761 1528 | 1573 | 1635 17 | 788 1700 | 1542 | 1584 | 1585 1561 | 1649 | 1508 1722 | 1687 1 | 654 1783 |
| 1476 1473 1515 | | | 1484 1463 | 1494 | 1545 148 | 1437 | 1480 | 1487 142 | 23 1490 | 1446 | | 1500 1545 | | | 08 1575 | | | 1467 15 | | | | | 1535 1567 | | | 1507 15 | | 1514 140 | 1514 | 1449 14 | | 1527 (| | 699 1609 | | 1607 19 | 570 1590 | 1580 | 1613 | 1598 1551 | 1568 | 1556 1605 | 1632 1 | 642 1620 |
| 1412 1488 1546 1470 1468 1577 | | | 1501 1574 1468 1577 | | 1537 1400 1497 1409 | 1468 | | 1539 146 1564 145 | | | | 1438 1566 1449 1475 | | | 19 1531 | | | | 68 1517 | | | | 1511 1597 1442 1462 | | | 1451 14 | | 1565 151 | | | | | | 506 1457 | | 1592 16 1684 16 | 655 1563 636 1515 | 1568 1614 | 1609 1 1657 1 | 1566 1504 | 1579 | 1561 1620 | 1666 1 | 581 1717 |
| 1470 1468 1522 1332 1498 1541 | | 2011 | 1468 15// 1510 1566 | 1355 | 1669 1441 | 15/6 | 1513 1531 | 1519 145 | 63 1535 66 1392 | 1576 | 1330 1 | 421 1614 | | 1463 14 | | 1439 | | 1377 15 1556 15 | | | | | 1442 1462 1564 1558 | | 1631 | | | 1408 133 1597 155 | | | 92 1372 77 1645 | 1589 1594 1377 1583 | 1584 1529 | | 1731 1689 | | 690 1701 | | 1618 | 1656 1485 | 1619 | 1000 IS/I 1438 1651 | 1697 1 | 470 1001 679 1665 |
| 1369 1515 1484 | | | 1548 1544 | 1325 | 1572 144 | 1480 | 1463 | 1475 153 | 32 1380 | 1610 | 1357 1 | 1376 1556 | | 1358 15 | | | | | | | | | | | | | | 1557 155 | | | 86 1607 | 1450 1611 | | | 0 | 1761 17 | | | 1597 | 1669 1597 | 1613 | 1526 1703 | 1575 1 | 643 1683 |
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| 1245 1224 1251 | 1 1304 | 1239 | 1243 1230 | 1228 | 1233 1200 | 1186 | 1219 | 1225 115 | 59 1260 | 1197 | 1224 1 | 1208 1287 | | | 01 1285 | | | 1192 12 | | | 1227 | | 1235 1278 | | | 1228 12 | 34 1261 | 1241 123 | 1238 | 1199 12 | 04 1235 | 1277 1261 | 1358 | 228 1263 | 1264 | 1254 | 0 1252 | | | 1329 1306 | 1251 | 1327 1289 | 1415 1 | 275 1309 |
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| 1335 1492 1516 1343 1563 1490 | | 1487 1498 | 14/4 1569 | 1348 | 1605 1435 | 1501 | 1524 | 1526 155 | ou 13/5 | 1592 | 1367 1 | 1468 1610 1305 1621 | | 1340 15 1357 15 | 5/ 1552 | 1552 1502 | 1521 1505 | | 24 1394 67 1451 | 4 1509 1 1486 | | | 1537 1589 1609 1495 | | | 1457 13 1460 14 | 86 1597 86 1618 | 1577 156 1587 155 | | 1461 15 1384 15 | | 1392 1584 1404 1589 | 1541 : | 509 1436 | 1530 | 1543 16 | 06/ 1645 701 1653 | 1/00 | 1/61 | 1689 1653 1765 1647 | 1657 | 1558 1705 | 1686 1 | 695 1691 677 1600 |
| 1303 1511 1486 | | | 1508 1587 | 1316 | 1586 130 | 1493 | 1547 | 1532 148 | 33 1417 | 1678 | 1343 1 | 1355 1051 1422 1614 | | 1355 15 | 91 1452 87 1522 | | | 1543 15 | | | | | | | | | | 1586 159 | | | | 1357 1633 | 1564 | 620 1488 | 1538 | 1571 17 | 701 1605 714 1622 | 1532 | 1596 | | | 1604 1750 | 1677 1 | 688 1740 |
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| 1428 1474 1487 | 7 1573 | 1499 | 1468 1552 | 1462 | 1548 144 | 1472 | 1500 | 1495 140 | 1475 | 1537 | 1464 1 | A56 1555 | 1446 | 1419 15 | 05 1571 | 1478 | | 1499 15 | | | | | 1522 1600 | | | 1506 15 | | 1503 151 | | 1451 14 | 51 1551 | 1511 1566 | 1551 | 608 1507 | 1514 | 1556 16 | 661 1593 | 1499 | 1588 | 1614 1506 | 0 | 1553 1762 | 1673 1 | 702 1665 |
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| 1470 1468 1504 | 4 1531 | 1544 | 1502 1515 | 1427 | 1532 149 | 1404 | 1508 | 1457 145 | 54 1495 | 1473 | 1434 1 | 1480 1585 | 1490 | 1456 14 | 58 1536 na 1536 | 1405 | 1533 | 1472 14 | 93 1499 or 1404 | 2 1457 | 1506 | 1557 | 1562 1507 | 1538 | 1603 | 1588 15 | 50 1508 | 1494 145 | 7 1509 | 1517 14 | 54 1507 | 1494 1577 | 1588 | 558 1470 | 1536 | 1559 16 | 659 1547 | 1574 | 1578 | 1543 1408 | 1547 | 1589 0 | 1651 1 | 723 1625 |
| 1414 1521 1435 1381 1535 1485 | 9 1565 5 1583 | 1504 | 1500 1497 | 1343 | 1572 146 | 1463 | 1463 | 1509 148 | 1426 | 1551 | 1400 1 | 1424 1546 1377 1557 | 1454 1575 | 1458 14 1446 14 | 97 1535 58 1588 | 1503 1509 | 1528 1491 | 1509 14 1463 14 | 86 1494 73 1528 | 4 1459 8 1456 | 1551 1604 | 1529 1546 | 1565 1561 1518 1475 | 1646 1609 | 1523 1557 | 1526 15 1502 15 | 13 1544 12 1614 | 1509 142 1531 147 | 18 1421 14 1450 | 1505 15 1444 14 | 05 1497 38 1474 | 1451 1610 1500 1613 | 1690 | .550 1501 .499 1517 | 1473 1552 | 1514 16 | DUD 1538 | 1545 | 1561 | 1505 1513 | 1551 1600 | 164 1565 | 1711 | 508 1715 0 1666 |
| 734 784 777 | 7 781 | 738 | 746 822 | 716 | 839 779 | 733 | 759 | 756 74 | 15 720 | 822 | 695 | | | | 10 753 | | 720 | | | | | | 795 734 | | | | | 795 79 | | | | | | 807 719 | | 796 9 | 909 759 | 776 | 776 | 822 732 | 778 | 766 751 | 856 | 784 0 |
| 1367 1419 1459 | 9 1494 | 1433 | 1483 1493 | 1366 | 1481 142 | 1380 | 1466 | 1463 139 | 9 1351 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 1513 | 1502 1448 | 1517 | 1539 1552 | | |
| | | | | | | | | | | | | | | | | | | | - " | | | | | | | - | - | | - | | | 27.0 | | | | | | | | | | | | |

Challenges using MPI

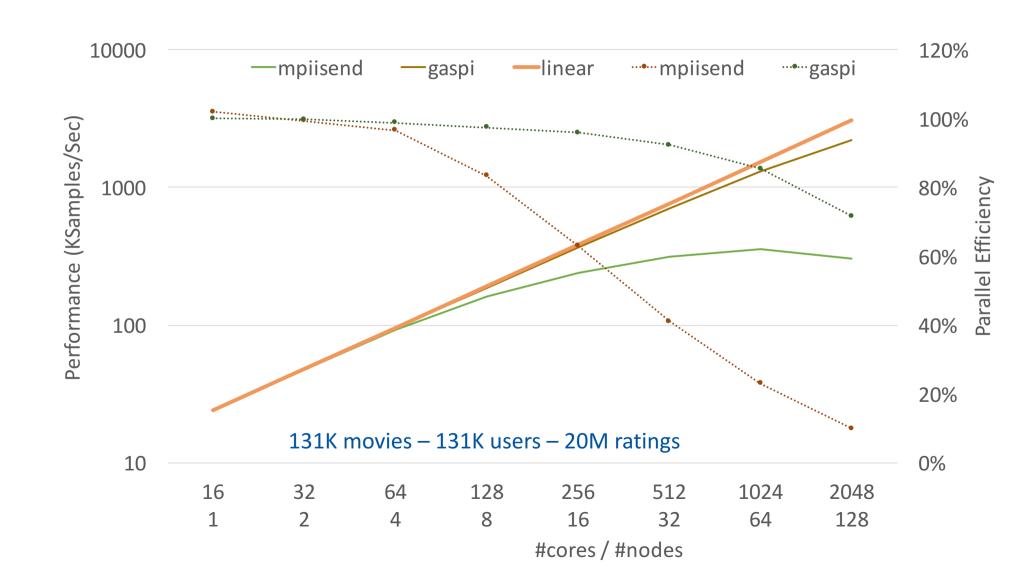
- MPI is not thread-safe by default
 - Multiple work threads, one MPI thread
- MPI calls have high overhead
 - Buffer before send
- Many possible MPI primitives
 - MPI_Bcast
 - simple, synchronous, does not scale well
 - MPI_Put:
 - need to split U in multiple MPI Windows, one window per peer
 - actual MPI work delayed until end of epoch
 - MPI_Isend/Irecv
 - best at doing background work
 - many irecvs/isends in flight

Current best MPI implementation

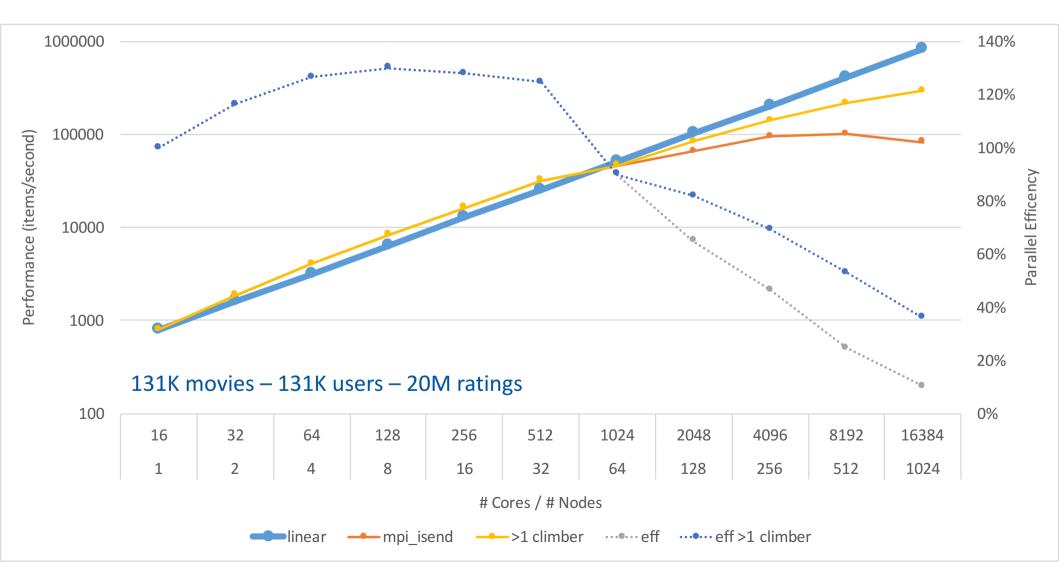
- Buffered ISend/IRecv
 - One buffer-pair per send-receive pair
 - Several chunks per buffer
 - Several items per chunk



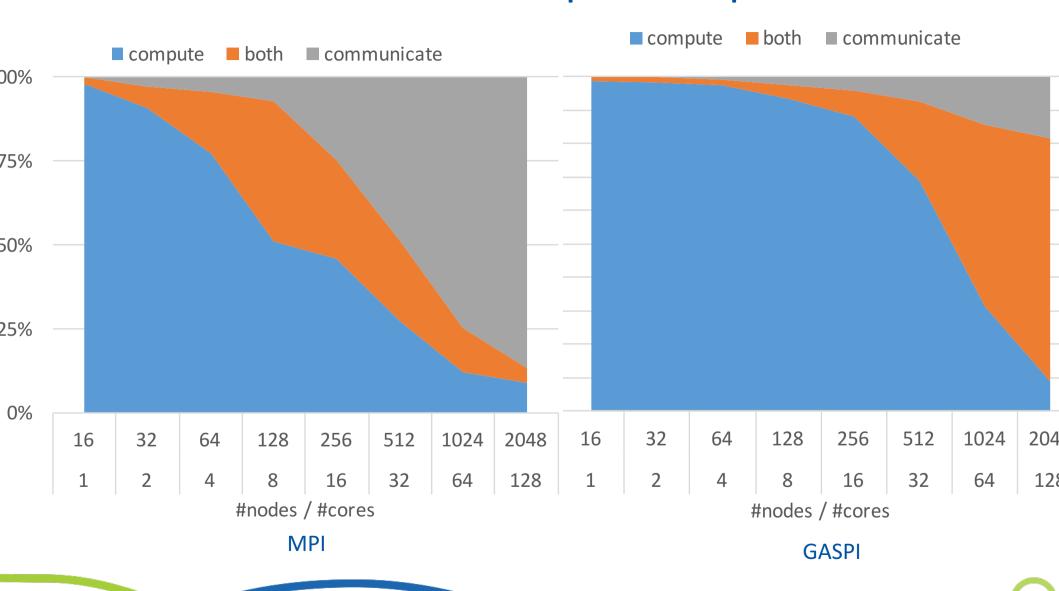
Distributed Performance – 128 nodes



Distributed Performance – 1K nodes



Comm – Comp Overlap



Conclusions optimizing BPMF

Reduce runtime on industrial data (estimated)

| Parallelism | Time 1 Run |
|---------------------------------|------------|
| Single node - Julia | 15 days |
| Single node - C++ & TBB | 1.5 hours |
| Distributed - C++ & TBB & GASPI | 5 minutes |

- Parallel efficiency is important
 - Load Balancing and Communication Hiding
- BPMF Released on GitHub
 - https://github.com/ExaScience/bpmf
 - https://github.com/jaak-s/BayesianDataFusion.jl