

Phase field models and their numerical methods

2. Energy stable numerical methods

August 14, 2019

Figure 11: $\beta_{\text{eff}} = 1.1$, $\beta_{\text{eff}} = 1.1$, $\beta_{\text{eff}} = 1.1$

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

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- Invariant energy quadratization (IEQ) schemes
- Scalar auxiliary variable (SAV) schemes

2.1.4.6 **ODE**

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model

11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1041 1042 1043 1044 10

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

- Invariant energy quadratization (IEQ) schemes
- Scalar auxiliary variable (SAV) schemes

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model

Allen-Cahn equation

Allen-Cahn equation:

$$u_t - \Delta u + \frac{1}{\varepsilon^2} f(u) = 0, \quad f(u) = F'(u) = u^3 - u. \quad (1)$$

L^2 gradient flow of the energy functional:

$$E(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u) \right) dx, \quad F(u) = \frac{1}{4} (u^2 - 1)^2. \quad (2)$$

Energy dissipation law (under suitable BCs):

$$\frac{dE}{dt} = -\|u_t\|^2. \quad (3)$$

1 Classic implicit-explicit methods

- Fully implicit schemes
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- Stabilization schemes

2 Energy quadratization methods

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First order scheme (continued)

Energy stability of (BE)

For $\Delta t \leq \varepsilon^2$, the BE scheme is energy stable:

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{1}{2\varepsilon^2}\right) \|u_{n+1} - u_n\|^2,$$

$$\text{where } E_n = E(u_n) = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2} \|u_n^2 - 1\|^2.$$

Proof. Take the inner product of (BE) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 + (\nabla u_{n+1}, \nabla u_{n+1} - \nabla u_n) + \frac{1}{\varepsilon^2} (f(u_{n+1}), u_{n+1} - u_n) = 0.$$

Since $2a(a - b) = a^2 - b^2 + (a - b)^2$, we have

$$(\nabla u_{n+1}, \nabla u_{n+1} - \nabla u_n) = \frac{1}{2} \|\nabla u_{n+1}\|^2 - \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{2} \|\nabla u_{n+1} - \nabla u_n\|^2.$$

$$(F(v) = F(w))$$

Second order scheme (continued)

Energy stability of (MCN)

For any $\Delta t > 0$, the MCN scheme is energy stable:

$$E_{n+1} - E_n = -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2,$$

$$\text{where } E_n = E(u_n) = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2} \|u_n^2 - 1\|^2.$$

Proof. Take the inner product of (MCN) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 + \frac{1}{2} (\|\nabla u_{n+1}\|^2 - \|\nabla u_n\|^2) + \frac{1}{\varepsilon^2} (\tilde{f}(u_{n+1}, u_n), u_{n+1} - u_n) = 0.$$

Since

$$(\tilde{f}(u_{n+1}, u_n), u_{n+1} - u_n) = (F(u_{n+1}) - F(u_n), 1),$$

we obtain

$$E_{n+1} - E_n = -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2. \quad \square$$

Remarks on the fully implicit schemes

Advantages:

- Easy to construct;
- Truncated error only comes from the approximation of u_t .

Disadvantages:

- $\Delta t \leq \varepsilon^2$ for unique solvability and energy stability;
- Nonlinearity leads to large amounts of computation.

References:

- Feng-Prohl, *Numer. Math.*, 2003.
- Du-Nicolaides, *SIAM J. Numer. Anal.*, 1991.

Outline

- 1 Classic implicit-explicit methods
 - Fully implicit schemes
 - Convex splitting schemes
 - Stabilization schemes
- 2 Energy quadratization methods
 - Invariant energy quadratization (IEQ) schemes
 - Scalar auxiliary variable (SAV) schemes
- 3 Exponential time differencing (ETD) methods
 - General theory for ODE systems
 - Example 1. Allen-Cahn equation
 - Example 2. No-slope-selection epitaxial growth model

$$E(\omega) = E_1(\omega) + E_2(\omega) + E_3(\omega)$$
$$E(u) - E_{\lambda}(u) = E_{\lambda}(u) - E(u) \quad (4)$$

1. *Journal of Management Studies*, 1997, 34, 1, 1-14.

First order scheme (continued)

Proof. Unique solvability. Define

$$\mathcal{E}(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{4\varepsilon^2} u^4 - \frac{1}{\varepsilon^2} u_n u + \frac{1}{2\Delta t} (u - u_n)^2 \right) dx.$$

First variational derivative of \mathcal{E} :

$$\frac{\delta \mathcal{E}(u)}{\delta u} = -\Delta u + \frac{1}{\varepsilon^2}(u^3 - u_n) + \frac{1}{\Delta t}(u - u_n).$$

Notice that (CS1) is equivalent to

$$\frac{\delta \mathcal{E}(u_{n+1})}{\delta u} = 0. \quad (5)$$

Second variational of \mathcal{E} :

$$\frac{d^2 \mathcal{E}(u + \lambda v)}{d\lambda^2} \Big|_{\lambda=0} = \int_{\Omega} \left(|\nabla v|^2 + \frac{3}{\varepsilon^2} u^2 v^2 + \frac{1}{\Delta t} v^2 \right) dx > 0, \quad \forall v \neq 0.$$

That is, \mathcal{E} is strictly convex and (CS1) is equivalent to

$$u_{n+1} = \operatorname{argmin} \mathcal{E}(v), \quad v \in H^1(\Omega).$$

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 - \frac{1}{2} \|\nabla u_{n+1} - \nabla u_n\|^2. \quad \square$$

Relation between the BE and CS1 schemes

The CS1 scheme can be rewritten as the fully implicit scheme

$$\frac{u_{n+1} - u_n}{\Delta t'} - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_{n+1}) = 0, \quad (6)$$

with different time step size $\Delta t' = \frac{\Delta t \varepsilon^2}{\Delta t + \varepsilon^2}$.

Proof. Note that

$$u_{n+1}^3 - u_n = u_{n+1}^3 - u_{n+1} + (u_{n+1} - u_n) = f(u_{n+1}) + (u_{n+1} - u_n).$$

Substitute the above identity into (CS1):

$$\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2} \right) (u_{n+1} - u_n) - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_{n+1}) = 0.$$

This is (6) with the time step $\Delta t'$ defined by $\frac{1}{\Delta t'} = \frac{1}{\Delta t} + \frac{1}{\varepsilon^2}$. □

Relation between the BE and CS1 schemes (continued)

- *Why is the CS1 scheme always energy stable?*

For any $\Delta t > 0$, since

$$\Delta t' = \frac{\Delta t \varepsilon^2}{\Delta t + \varepsilon^2} < \varepsilon^2,$$

the fully implicit scheme (6) is energy stable.

- *Existence of a time-delay.*

Denote by $u^{\text{BE}}(t_n)$ and $u^{\text{CS}}(t_n)$ the solutions to (BE) and (CS1).

Then,

$$u^{\text{CS}}(t_n) = u^{\text{BE}}(\delta t_n), \quad \delta = \frac{\varepsilon^2}{\Delta t + \varepsilon^2} < 1.$$

A larger time step size Δt , giving a smaller δ , leads to a more significant time-delay. Such a delay will diminish as $\Delta t \rightarrow 0$.

Second order scheme

The second order convex splitting (CS2) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} - \Delta \frac{u_{n+1} + u_n}{2} + \frac{1}{\varepsilon^2} \left(\tilde{f}_+(u_{n+1}, u_n) - \left(\frac{3}{2}u_n - \frac{1}{2}u_{n-1} \right) \right) = 0. \quad (\text{CS2})$$

Theorem: Energy stability of (CS2)

For any $\Delta t > 0$, the CS2 scheme is energy stable:

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2,$$

where E_n is a modification of $E(u_n)$:

$$E_n = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2} \|u_n^2 - 1\|^2 + \frac{1}{4\varepsilon^2} \|u_n - u_{n-1}\|^2.$$

Second order scheme (continued)

Energy stability of (CS2)

For any $\Delta t > 0$, the CS2 scheme is energy stable:

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2,$$

$$\text{where } E_n = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2} \|u_n^2 - 1\|^2 + \frac{1}{4\varepsilon^2} \|u_n - u_{n-1}\|^2.$$

Proof. Take the inner product of (CS2) with $u_{n+1} - u_n$:

$$\begin{aligned} & \frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 + \frac{1}{2} (\|\nabla u_{n+1}\|^2 - \|\nabla u_n\|^2) \\ & + \frac{1}{\varepsilon^2} (\tilde{f}_+(u_{n+1}, u_n), u_{n+1} - u_n) - \frac{1}{\varepsilon^2} \left(\frac{3}{2} u_n - \frac{1}{2} u_{n-1}, u_{n+1} - u_n \right) = 0, \end{aligned}$$

where

$$(\tilde{f}_+(u_{n+1}, u_n), u_{n+1} - u_n) = (F_+(u_{n+1}) - F_+(u_n), 1).$$

we have

Then, we obtain

that is,

$$E_{n+1} - E_n = -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 - \frac{1}{4\varepsilon^2} \|u_{n+1} - 2u_n + u_{n-1}\|^2. \quad \square$$

Remarks on the convex splitting schemes

Advantages:

- Easy to construct;
- **Unconditional** unique solvability and energy stability (1st order);
- Easy to prove the energy stability.

Disadvantages:

- Existence of the time-delay may cause more truncated errors;
- Nonlinearity leads to large amounts of computation;
- Hard to obtain the energy stability for higher order schemes.

References:

- David J. Eyre, a note, 1997.
- Shen-Wang-Wang-Wise, *SIAM J. Numer. Anal.*, 2012.
- Xu-Li-Wu, *arXiv:1604.05402v4*, 2017.

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First order scheme (continued)

Theorem: Energy stability of (STAB1)

Denote $L = \|f'\|_{L^\infty}$ and assume that $L < \infty$.

(i) For $S = 0$ and $\Delta t \leq \frac{2\varepsilon^2}{L}$, the STAB1 scheme is energy stable:

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{L}{2\varepsilon^2}\right) \|u_{n+1} - u_n\|^2;$$

(ii) For $S \geq \frac{L}{2}$ and $\Delta t > 0$, the STAB1 scheme is energy stable:

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{\varepsilon^2} (F(u_n), 1)$.

Then, $E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2} - \frac{L}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2.$

First order scheme (continued)

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2} - \frac{L}{2\varepsilon^2}\right) \|u_{n+1} - u_n\|^2.$$

For (i), when $S = 0$, we have

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{L}{2\varepsilon^2}\right) \|u_{n+1} - u_n\|^2.$$

The condition $\Delta t \leq \frac{2\varepsilon^2}{L}$ leads to the energy stability.

For (ii), when $S \geq \frac{L}{2}$, we have

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2.$$

Energy stability holds for any $\Delta t > 0$.



First order scheme (continued)

A question is whether $\|f'\|_{L^\infty}$ is finite.

In fact, we have the following result:

For the Allen-Cahn equation, if $u(0) \in [-1, 1]$ a.e., then $u(t) \in [-1, 1]$ a.e. for any $t > 0$.

For a large positive number $M \gg 1$, we modify the potential $F(u)$ as

$$\tilde{F}(u) = \begin{cases} \frac{1}{4}(u^2 - 1)^2, & |u| \leq M, \\ au^2 + bu + c, & |u| > M, \end{cases}$$

where $a, b, c \in \mathbb{R}$ are chosen such that $\tilde{F} \in C^2(\mathbb{R})$, and define $\tilde{f}(u) = \tilde{F}'(u)$. If we denote $L = \|\tilde{f}'\|_{L^\infty}$, then L must be a finite number.

Relation between the STAB1 and CS1 schemes

Consider the splitting form $F(u) = F_+(u) - F_-(u)$ with

$$F_+(u) = \frac{S}{2}u^2 + \frac{1}{4}, \quad F_-(u) = \frac{S+1}{2}u^2 - \frac{1}{4}u^4, \quad S \geq 0.$$

Here,

- F_+ is always convex in \mathbb{R} ;
- F_- is convex on $[-1, 1]$ when $S \geq 2$.

The corresponding convex splitting scheme reads

$$\frac{u_{n+1} - u_n}{\Delta t} - \Delta u_{n+1} + \frac{S}{\varepsilon^2} u_{n+1} - \frac{1}{\varepsilon^2} (S u_n - f(u_n)) = 0,$$

which is exactly the STAB1 scheme.

Second order scheme

Second order BDF-type stabilization (STAB-BDF2) scheme:

$$\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} - \Delta u_{n+1} + \frac{1}{\varepsilon^2} (2f(u_n) - f(u_{n-1})) + \frac{S}{\varepsilon^2} (u_{n+1} - 2u_n + u_{n-1})$$

(STAB-BDF2)

Theorem: Energy stability of (STAB-BDF2)

Denote $L = \|f'\|_{L^\infty}$ and assume that $L < \infty$.

For $S \geq 0$ and $\Delta t \leq \frac{2\varepsilon^2}{3L}$, the STAB-BDF2 scheme is energy stable:

$$E_{n+1} \leq E_n,$$

where

$$E_n = \frac{1}{2} \|\nabla u_n\|^2 + \frac{1}{\varepsilon^2} (F(u_n), 1) + \left(\frac{1}{4\Delta t} + \frac{S+L}{2\varepsilon^2} \right) \|u_n - u_{n-1}\|^2.$$

0

- Easy to construct;
- **Unconditional** unique solvability and energy stability (1st order);
- Linear scheme with constant coefficient, so we can use FFT.

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- Stabilization term introduces an extra truncated error;
- Theoretically, $\|f'(u)\|_{L^\infty} < \infty$ does not hold for general cases, unless we know $\|u\|_{L^\infty} \leq C$ for some certain C ;
- Hard to obtain the energy stability for higher order schemes.

- Shen-Yang, *Discrete Contin. Dyn. Syst.*, 2010.

11 12 13 14 15

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

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- Invariant energy quadratization (IEQ) schemes
- Scalar auxiliary variable (SAV) schemes

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model



Gradient flow and energy functional

Gradient flow:

$$\frac{\partial u}{\partial t} = G\mu, \quad \mu = \frac{\delta E}{\delta u}. \quad (7)$$

Energy dissipation law:

$$\frac{dE}{dt} = \left(\frac{\delta E}{\delta u}, \frac{\partial u}{\partial t} \right) = (\mu, G\mu) \leq 0.$$

Energy functional:

$$E(u) = \frac{1}{2}(u, Lu) + E_1(u), \quad (8)$$

- G is self-adjoint and *negative definite*;
- L is self-adjoint and *positive semi-definite*;
- E_1 is nonlinear but with lower order derivatives than L and *bounded from below*.

The gradient flow (7) equipped with the energy (8) reads

$$u_t = G\mu, \quad \mu = Lu + N(u), \quad N(u) = \frac{\delta E_1}{\delta u}. \quad (9)$$

Outline

- 1 Classic implicit-explicit methods
 - Fully implicit schemes
 - Convex splitting schemes
 - Stabilization schemes
- 2 Energy quadratization methods
 - Invariant energy quadratization (IEQ) schemes
 - Scalar auxiliary variable (SAV) schemes
- 3 Exponential time differencing (ETD) methods
 - General theory for ODE systems
 - Example 1. Allen-Cahn equation
 - Example 2. No-slope-selection epitaxial growth model

Equivalent forms (continued)

$$\frac{d}{dt} \tilde{E}(u, q) = (\mu, G\mu) \leq 0.$$

Proof. Take the inner product of (10a) with μ :

$$(\mu, u_t) = (\mu, G\mu).$$

Take the inner product of (10b) with u_t :

$$(\mu, u_t) = (Lu, u_t) + \left(\frac{N(u)}{\sqrt{F(u)}} q, u_t \right).$$

Take the inner product of (10c) with $2q$:

$$2(q, q_t) = \left(\frac{N(u)}{\sqrt{F(u)}} u_t, q \right).$$

Then, we obtain

$$(\mu, G\mu) = (Lu, u_t) + 2(q, q_t) = \frac{d}{dt} \left(\frac{1}{2} (u, Lu) + \|q\|^2 \right). \quad \square$$

First order IEQ scheme

Gradient flow:

$$\begin{aligned}u_t &= G\mu, \\ \mu &= Lu + \frac{q}{\sqrt{F(u)}}N(u), \\ q_t &= \frac{N(u)}{2\sqrt{F(u)}}u_t.\end{aligned}$$

First order IEQ (IEQ1) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1}, \tag{12a}$$

$$\mu_{n+1} = Lu_{n+1} + \frac{q_{n+1}}{\sqrt{F(u_n)}}N(u_n), \tag{12b}$$

$$\frac{q_{n+1} - q_n}{\Delta t} = \frac{N(u_n)}{2\sqrt{F(u_n)}} \frac{u_{n+1} - u_n}{\Delta t}. \tag{12c}$$

IEQ1 scheme: Unique solvability (continued)

For any $\Delta t > 0$, the IEQ1 scheme admits a unique solution.

IEQ1 scheme (denote $b_n = \frac{N(u_n)}{\sqrt{F(u_n)}}$):

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1},$$

$$\mu_{n+1} = Lu_{n+1} + q_{n+1}b_n,$$

$$q_{n+1} - q_n = \frac{1}{2}b_n(u_{n+1} - u_n).$$

Proof. Eliminate μ_{n+1} and q_{n+1} :

$$\frac{u_{n+1} - u_n}{\Delta t} = GLu_{n+1} + G(q_nb_n) + \frac{1}{2}G(b_n^2u_{n+1}) - \frac{1}{2}G(b_n^2u_n),$$

or equivalently,

$$u_{n+1} - \Delta t GLu_{n+1} - \frac{\Delta t}{2}G(b_n^2u_{n+1}) = u_n + \Delta t G(q_nb_n) - \frac{\Delta t}{2}G(b_n^2u_n) =: c_n.$$

IEQ1 scheme: Unique solvability (continued)

$$u_{n+1} - \Delta t GLu_{n+1} - \frac{\Delta t}{2} G(b_n^2 u_{n+1}) = c_n.$$

Act G^{-1} on both sides:

$$\left(G^{-1} - \Delta t L - \frac{\Delta t}{2} b_n^2 I\right) u_{n+1} = G^{-1} c_n.$$

Here, $G^{-1} - \Delta t L - \frac{\Delta t}{2} b_n^2 I$ is negative definite. □

Algorithm: IEQ1 scheme

Given u_n, q_n , to compute u_{n+1}, q_{n+1} as follows:

- ① Calculate b_n and c_n ;
- ② Solve $(I - \Delta t GL)u_{n+1} - \frac{\Delta t}{2} G(b_n^2 u_{n+1}) = c_n$ to obtain u_{n+1} ;
- ③ Calculate q_{n+1} by $q_{n+1} = q_n + \frac{1}{2} b_n (u_{n+1} - u_n)$.

IEQ1 scheme: Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0$,
 where $E_n = \tilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + \|q_n\|^2$.

Proof. Take the inner product of (12a) with $\Delta t\mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t(\mu_{n+1}, G\mu_{n+1}).$$

Take the inner product of (12b) with $u_{n+1} - u_n$:

$$(\mu_{n+1}, u_{n+1} - u_n) = (Lu_{n+1}, u_{n+1} - u_n) + (q_{n+1}b_n, u_{n+1} - u_n).$$

Take the inner product of (12c) with $2q_{n+1}$:

$$(2q_{n+1}, q_{n+1} - q_n) = (q_{n+1}b_n, u_{n+1} - u_n).$$

Then, we obtain

$$E_{n+1} - E_n + \frac{1}{2}(L(u_{n+1} - u_n), u_{n+1} - u_n) + \|q_{n+1} - q_n\|^2 = \Delta t(\mu_{n+1}, G\mu_{n+1}).$$

Remark. Generally, $q_n \neq \sqrt{F(u_n)}$, so $E_n \neq E(u_n)$.

Second order IEQ scheme: IEQ-CN

$$\begin{aligned}
 u_t &= G\mu, \\
 \mu &= Lu + \frac{q}{\sqrt{F(u)}}N(u), \\
 q_t &= \frac{N(u)}{2\sqrt{F(u)}}u_t.
 \end{aligned}$$

Crank-Nicolson-type IEQ (IEQ-CN) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+\frac{1}{2}}, \quad (13a)$$

$$\mu_{n+\frac{1}{2}} = \frac{1}{2}L(u_{n+1} + u_n) + \frac{q_{n+1} + q_n}{2}\bar{b}_{n+\frac{1}{2}}, \quad (13b)$$

$$\frac{q_{n+1} - q_n}{\Delta t} = \frac{1}{2}\bar{b}_{n+\frac{1}{2}}\frac{u_{n+1} - u_n}{\Delta t}, \quad (13c)$$

where $\bar{b}_{n+\frac{1}{2}} = \frac{3}{2}b_n - \frac{1}{2}b_{n-1}$ with $b_n = \frac{N(u_n)}{\sqrt{F(u_n)}}$.

Second order IEQ scheme: IEQ-CN (continued)

Unique solvability

For any $\Delta t > 0$, the IEQ-CN scheme admits a unique solution.

Energy stability

For any $\Delta t > 0$, the IEQ-CN scheme is energy stable:

$$E_{n+1} - E_n = \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where $E_n = \tilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + \|q_n\|^2$.

Proof. Taking the inner products of (13a), (13b), (13c) with $\Delta t \mu_{n+\frac{1}{2}}$, $-(u_{n+1} - u_n)$, $\Delta t(q_{n+1} + q_n)$, respectively, and adding the resulted three equalities yield the expected result. \square



Second order IEQ scheme: IEQ-BDF2

$$\begin{aligned}
 u_t &= G\mu, \\
 \mu &= Lu + \frac{q}{\sqrt{F(u)}}N(u), \\
 q_t &= \frac{N(u)}{2\sqrt{F(u)}}u_t.
 \end{aligned}$$

Second order BDF-type IEQ (IEQ-BDF2) scheme:

$$\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} = G\mu_{n+1}, \quad (14a)$$

$$\mu_{n+1} = Lu_{n+1} + q_{n+1}\bar{b}_{n+1}, \quad (14b)$$

$$\frac{3q_{n+1} - 4q_n + q_{n-1}}{2\Delta t} = \frac{1}{2}\bar{b}_{n+1}\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t}, \quad (14c)$$

where $\bar{b}_{n+1} = 2b_n - b_{n-1}$.

1. *Journal of Management Studies*, 1997, 34, 1, 1-14.

10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 | 90 | 100

1 1 1

[illegible]

- Linear scheme and unique solvability;
- Unconditional energy stability (w.r.t. a modified energy);
- Easy to construct higher order schemes;

- Linear system with variable coefficient, cannot use FFT;
- For some problems, $F(u)$ is not bounded from below.

- XF Yang et al, *J. Comput. Phys.*, 2016-2017.

[illegible]

Equivalent energy:

$$\tilde{E}(u, q) = \int \left(\frac{1}{4} q^2 + \frac{1-\varepsilon}{2} u^2 - |\nabla u|^2 + \frac{1}{2} |\Delta u|^2 \right) dx.$$

Equivalent equation:

$$u_t = \Delta \mu,$$

$$\mu = qu + (1 - \varepsilon)u + 2\Delta u + \Delta^2 u,$$

$$q_t = 2uu_t.$$

IEQ1 scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = \Delta \mu_{n+1}, \quad (15a)$$

$$\mu_{n+1} = q_{n+1}u_n + (1 - \varepsilon)u_{n+1} + 2\Delta u_n + \Delta^2 u_{n+1}, \quad (15b)$$

$$q_{n+1} - q_n = 2u_n(u_{n+1} - u_n). \quad (15c)$$

Example 1. Phase field crystal model (continued)

Energy stability (Note that $q_n \neq u_n^2$, so $E_n \neq E(u_n)$.)

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq -\Delta t \|\nabla \mu_{n+1}\|^2 \leq 0$,
 where $E_n = \tilde{E}(u_n, q_n) = \frac{1}{4} \|q_n\|^2 + \frac{1-\varepsilon}{2} \|u_n\|^2 - \|\nabla u_n\|^2 + \frac{1}{2} \|\Delta u_n\|^2$.

Proof. Take the inner product of (15a) with $\Delta t \mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t (\mu_{n+1}, \Delta \mu_{n+1}) = -\Delta t \|\nabla \mu_{n+1}\|^2.$$

Take the inner product of (15b) with $u_{n+1} - u_n$:

$$\begin{aligned} (\mu_{n+1}, u_{n+1} - u_n) &= (q_{n+1} u_n, u_{n+1} - u_n) + (1 - \varepsilon) (u_{n+1}, u_{n+1} - u_n) \\ &\quad - 2(\nabla u_n, \nabla u_{n+1} - \nabla u_n) + (\Delta u_{n+1}, \Delta u_{n+1} - \Delta u_n). \end{aligned}$$

Take the inner product of (15c) with $\frac{1}{2} q_{n+1}$:

$$\frac{1}{2} (q_{n+1}, q_{n+1} - q_n) = (q_{n+1} u_n, u_{n+1} - u_n).$$

Just use the identities $a(a - b) = \dots$ and $b(a - b) = \dots$.



Example 2. No-slope-selection epitaxial growth

Epitaxial growth model without slope selection:

$$u_t = -\nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2} \right) - \varepsilon^2 \Delta^2 u, \quad (16)$$

Energy functional:

$$E(u) = \int \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) dx. \quad (17)$$

Strictly speaking, the IEQ method cannot be applied on this model since $-\frac{1}{2} \ln(1 + |\nabla u|^2)$ is *unbounded from below*. However, the basic idea could be used to construct an IEQ-like scheme.

Example 2. No-slope-selection epitaxial growth (continued)

Introduce an auxiliary variable $q = \sqrt{\ln(1 + |\nabla u|^2) + A}$, $\forall A > 0$.

Equivalent equation:

$$u_t = -\varepsilon^2 \Delta^2 u - \nabla \cdot (q \mathbf{v}), \quad (18a)$$

$$q_t = \mathbf{v} \cdot \nabla u_t, \quad (18b)$$

where

$$\mathbf{v} = \frac{\nabla u}{(1 + |\nabla u|^2) \sqrt{\ln(1 + |\nabla u|^2) + A}}.$$

Equivalent energy:

$$\tilde{E}(u, q) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\Delta u|^2 - \frac{1}{2} q^2 + \frac{1}{2} A \right) dx.$$

Taking the inner products of (18a) and (18b) with u_t and $-q$, and adding the resulted two equalities yield the energy dissipation law:

$$\frac{d}{dt} \tilde{E}(u, q) = -\|u_t\|^2 \leq 0.$$

Example 2. No-slope-selection epitaxial growth (continued)

Equivalent equation:

$$\begin{aligned}u_t &= -\varepsilon^2 \Delta^2 u - \nabla \cdot (q \mathbf{v}), \\q_t &= \mathbf{v} \cdot \nabla u_t,\end{aligned}$$

where

$$\mathbf{v} = \frac{\nabla u}{(1 + |\nabla u|^2) \sqrt{\ln(1 + |\nabla u|^2) + A}}.$$

First order scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = -\varepsilon^2 \Delta^2 u_{n+1} - \nabla \cdot (q_n \mathbf{v}_n), \quad (19a)$$

$$q_{n+1} - q_n = \mathbf{v}_n \cdot (\nabla u_{n+1} - \nabla u_n), \quad (19b)$$

where

$$\mathbf{v}_n = \frac{\nabla u_n}{(1 + |\nabla u_n|^2) \sqrt{\ln(1 + |\nabla u_n|^2) + A}}.$$

Example 2. No-slope-selection epitaxial growth (continued)

Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2$,
 where $E_n = \tilde{E}(u_n, q_n) = \frac{\varepsilon^2}{2} \|\Delta u_n\|^2 - \frac{1}{2} \|q_n\|^2 + \frac{1}{2} A |\Omega|$.

Proof. Take the inner product of (19a) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2 = -\varepsilon^2 (\Delta u_{n+1}, \Delta u_{n+1} - \Delta u_n) + (q_n \mathbf{v}_n, \nabla u_{n+1} - \nabla u_n).$$

Take the inner product of (19b) with q_n :

$$(q_n, q_{n+1} - q_n) = (q_n \mathbf{v}_n, \nabla u_{n+1} - \nabla u_n).$$

Then, we obtain

$$E_{n+1} - E_n + \frac{\varepsilon^2}{2} \|\Delta u_{n+1} - \Delta u_n\|^2 + \frac{1}{2} \|q_{n+1} - q_n\|^2 = -\frac{1}{\Delta t} \|u_{n+1} - u_n\|^2. \quad \square$$

Remark. Generally, $q_n \neq \sqrt{\ln(1 + |\nabla u_n|^2) + A}$, so $E_n \neq E(u_n)$.

1 Classic implicit-explicit methods

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

2 Energy quadratization methods

- Invariant energy quadratization (IEQ) schemes
- **Scalar auxiliary variable (SAV) schemes**

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model

Equivalent forms

Without loss of generality, we assume $E_1(u) > 0$.

Introduce a Scalar Auxiliary Variable $r(t) = \sqrt{E_1(u(t))}$.

Equivalent form of the gradient flow:

$$u_t = G\mu, \quad (20a)$$

$$\mu = Lu + \frac{r}{\sqrt{E_1(u)}} N(u), \quad (20b)$$

$$r_t = \frac{1}{2\sqrt{E_1(u)}} \int N(u) u_t \, dx. \quad (20c)$$

Equivalent form of the energy:

$$\tilde{E}(u, r) = \frac{1}{2}(u, Lu) + r^2. \quad (21)$$

Equivalent forms (continued)

$$\frac{d}{dt} \tilde{E}(u, r) = (\mu, G\mu) \leq 0.$$

Proof. Take the inner product of (20a) with μ :

$$(\mu, u_t) = (\mu, G\mu).$$

Take the inner product of (20b) with u_t :

$$(\mu, u_t) = (Lu, u_t) + \frac{r}{\sqrt{E_1(u)}} (N(u), u_t).$$

Multiply (20c) by $2r$:

$$2rr_t = \frac{r}{\sqrt{E_1(u)}} \int N(u) u_t \, dx.$$

Then, we obtain

$$(\mu, G\mu) = (Lu, u_t) + 2rr_t = \frac{d}{dt} \left(\frac{1}{2} (u, Lu) + r^2 \right) = \frac{d}{dt} \tilde{E}(u, r). \quad \square$$

First order SAV scheme

Gradient flow:

$$u_t = G\mu,$$

$$\mu = Lu + \frac{r}{\sqrt{E_1(u)}}N(u),$$

$$r_t = \frac{1}{2\sqrt{E_1(u)}} \int N(u)u_t \, dx.$$

First order SAV (SAV1) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1}, \quad (22a)$$

$$\mu_{n+1} = Lu_{n+1} + \frac{r_{n+1}}{\sqrt{E_1(u_n)}}N(u_n), \quad (22b)$$

$$\frac{r_{n+1} - r_n}{\Delta t} = \frac{1}{2\sqrt{E_1(u_n)}} \int N(u_n) \frac{u_{n+1} - u_n}{\Delta t} \, dx. \quad (22c)$$

SAV1 scheme: Unique solvability

For any $\Delta t > 0$, the SAV1 scheme admits a unique solution.

SAV1 scheme (denote $b_n = \frac{N(u_n)}{\sqrt{E_1(u_n)}}$):

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1},$$

$$\mu_{n+1} = Lu_{n+1} + r_{n+1}b_n,$$

$$r_{n+1} - r_n = \frac{1}{2}(b_n, u_{n+1} - u_n).$$

Proof. Eliminate μ_{n+1} and r_{n+1} :

$$\frac{u_{n+1} - u_n}{\Delta t} = GLu_{n+1} + r_n Gb_n + \frac{1}{2}(b_n, u_{n+1})Gb_n - \frac{1}{2}(b_n, u_n)Gb_n,$$

or equivalently,

$$u_{n+1} - \Delta t GLu_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1})Gb_n = u_n + \Delta tr_n Gb_n - \frac{\Delta t}{2}(b_n, u_n)Gb_n =: c_n.$$

[illegible]

$$u_{n+1} - \Delta t GLu_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1})Gb_n = c_n.$$

Act $(I - \Delta t GL)^{-1}$ on both sides:

$$u_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1})(I - \Delta t GL)^{-1}Gb_n = (I - \Delta t GL)^{-1}c_n.$$

Take the inner product with b_n :

$$(b_n, u_{n+1}) - \frac{\Delta t}{2}(b_n, u_{n+1})(b_n, (I - \Delta t GL)^{-1} G b_n) = (b_n, (I - \Delta t GL)^{-1} c_n),$$

or equivalently,

$$\left[1 - \frac{\Delta t}{2}(b_n, (I - \Delta t GL)^{-1} G b_n)\right](b_n, u_{n+1}) = (b_n, (I - \Delta t GL)^{-1} c_n).$$

Here, $(I - \Delta t GL)^{-1}G = (G^{-1} - \Delta t L)^{-1}$ is negative definite.



SAV1 scheme: Algorithm

Algorithm: SAV1 scheme

Given u_n, r_n , to compute u_{n+1}, r_{n+1} as follows:

- ① Calculate $b_n, (b_n, u_n), Gb_n$, and c_n ;
- ② Solve $(I - \Delta t GL)\theta_1 = Gb_n$ and $(I - \Delta t GL)\theta_2 = c_n$ to get θ_1, θ_2 ;
- ③ Calculate (b_n, u_{n+1}) by $(b_n, u_{n+1}) = \frac{(b_n, \theta_2)}{1 - \frac{\Delta t}{2}(b_n, \theta_1)}$;
- ④ Calculate u_{n+1} by $u_{n+1} = \frac{\Delta t}{2}(b_n, u_{n+1})\theta_1 + \theta_2$;
- ⑤ Calculate r_{n+1} by $r_{n+1} = r_n + \frac{1}{2}(b_n, u_{n+1}) - \frac{1}{2}(b_n, u_n)$.

SAV1 scheme: Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0$,
 where $E_n = \tilde{E}(u_n, r_n) = \frac{1}{2}(u_n, Lu_n) + r_n^2$.

Proof. Take the inner product of (22a) with $\Delta t\mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t(\mu_{n+1}, G\mu_{n+1}).$$

Take the inner product of (22b) with $u_{n+1} - u_n$:

$$(\mu_{n+1}, u_{n+1} - u_n) = (Lu_{n+1}, u_{n+1} - u_n) + r_{n+1}(b_n, u_{n+1} - u_n).$$

Multiply (22c) by $2r_{n+1}$:

$$2r_{n+1}(r_{n+1} - r_n) = r_{n+1}(b_n, u_{n+1} - u_n).$$

Then, we obtain

$$E_{n+1} - E_n + \frac{1}{2}(L(u_{n+1} - u_n), u_{n+1} - u_n) + (r_{n+1} - r_n)^2 = \Delta t(\mu_{n+1}, G\mu_{n+1}). \quad \square$$

Second order SAV scheme: SAV-CN

$$\begin{aligned}
 u_t &= G\mu, \\
 \mu &= Lu + \frac{r}{\sqrt{E_1(u)}}N(u), \\
 r_t &= \frac{1}{2\sqrt{E_1(u)}} \int N(u)u_t \, dx.
 \end{aligned}$$

Crank-Nicolson-type SAV (SAV-CN) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+\frac{1}{2}}, \quad (23a)$$

$$\mu_{n+\frac{1}{2}} = \frac{1}{2}L(u_{n+1} + u_n) + \frac{r_{n+1} + r_n}{2\sqrt{E_1(\bar{u}_{n+\frac{1}{2}})}}N(\bar{u}_{n+\frac{1}{2}}), \quad (23b)$$

$$\frac{r_{n+1} - r_n}{\Delta t} = \frac{1}{2\sqrt{E_1(\bar{u}_{n+\frac{1}{2}})}} \int N(\bar{u}_{n+\frac{1}{2}}) \frac{u_{n+1} - u_n}{\Delta t} \, dx, \quad (23c)$$

where $\bar{u}_{n+\frac{1}{2}}$ is an approximation of $u(t_{n+\frac{1}{2}})$ with error $\mathcal{O}(\Delta t^2)$.

Second order SAV scheme: SAV-CN (continued)

Unique solvability

For any $\Delta t > 0$, the SAV-CN scheme admits a unique solution.

Energy stability

For any $\Delta t > 0$, the SAV-CN scheme is energy stable:

$$E_{n+1} - E_n = \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where $E_n = \tilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + r_n^2$.

Second order SAV scheme: SAV-BDF2

$$\begin{aligned}
 u_t &= G\mu, \\
 \mu &= Lu + \frac{r}{\sqrt{E_1(u)}} N(u), \\
 r_t &= \frac{1}{2\sqrt{E_1(u)}} \int N(u) u_t \, dx.
 \end{aligned}$$

Second order BDF-type SAV (SAV-BDF2) scheme:

$$\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} = G\mu_{n+1}, \quad (24a)$$

$$\mu_{n+1} = Lu_{n+1} + \frac{r_{n+1}}{\sqrt{E_1(\bar{u}_{n+1})}} N(\bar{u}_{n+1}), \quad (24b)$$

$$\frac{3r_{n+1} - 4r_n + r_{n-1}}{2\Delta t} = \frac{1}{2\sqrt{E_1(\bar{u}_{n+1})}} \int N(\bar{u}_{n+1}) \frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} \, dx, \quad (24c)$$

where \bar{u}_{n+1} is an approximation of $u(t_{n+1})$ with error $\mathcal{O}(\Delta t^2)$.

- Shen Yu Yang / J Comput Phys 2017

- Shen-Xu-Yang, *J. Comput. Phys.*, 2017.

- 21 XX XX XX 1410 01001 1 0014

- Shen-Xu-Yang, *arXiv:1710.01331v1*, 2017.

Example 1. Fractional Cahn-Hilliard equation

Consider the fractional Cahn-Hilliard equation

$$u_t = -(-\Delta)^\alpha(-\Delta u + \frac{1}{\varepsilon^2}(u^3 - u)), \quad 0 \leq \alpha \leq 1, \quad (25)$$

which is the $H^{-\alpha}$ gradient flow of the energy

$$E(u) = \int \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{4\varepsilon^2} (u^2 - 1)^2 \right) dx. \quad (26)$$

We write the energy (26) in the form (8) by specifying

$$G = -(-\Delta)^\alpha, \quad L = -\Delta + \frac{S}{\varepsilon^2}, \quad E_1(u) = \frac{1}{4\varepsilon^2} \int (u^2 - 1 - S)^2 \, dx,$$

where $S > 0$ is a constant. Then, we have

$$N(u) = \frac{\delta E_1}{\delta u} = \frac{1}{\varepsilon^2} u(u^2 - 1 - S).$$

Example 2. No-slope-selection epitaxial growth

Consider the L^2 gradient flow of the energy

$$E(u) = \int \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) dx. \quad (27)$$

- IEQ method cannot be used.
- $\forall \alpha_0 > 0, \exists C_0 > 0$ s.t. $\forall \alpha > \alpha_0$, it holds

$$\int \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\alpha}{2} |\Delta u|^2 \right) dx \geq -C_0.$$

Choosing $\alpha \in (\alpha_0, \varepsilon^2)$, we write the energy (27) in the form (8) by specifying $G = -I$, $L = (\varepsilon^2 - \alpha)\Delta^2$, and

$$E_1(u) = \int \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\alpha}{2} |\Delta u|^2 \right) dx.$$

Fig. 11. σ_{eff} vs. σ_{eff}^0 for $\sigma_{\text{eff}}^0 = 1$.

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

- Invariant energy quadratization (IEQ) schemes
- Scalar auxiliary variable (SAV) schemes

Q14. What is the order of the ODE?

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model

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- General theory for ODE systems
- Example 1. Allen-Cahn equation
- Example 2. No-slope-selection epitaxial growth model

From PDE to ODE system

Consider the PDE for a scalar function $u : \overline{\Omega} \times [0, \infty) \rightarrow \mathbb{R}$ as

$$u_t = \mathcal{L}u + \mathcal{N}(u), \quad (28)$$

where

- \mathcal{L} is a linear, self-adjoint, and negative definite operator;
- \mathcal{N} denotes a generic nonlinear term.

Discretizing the PDE (28) in spatial variables (for instance, by spectral or finite difference approximations) often leads to a system of ODEs:

$$u_t + \mathbf{L}u = \mathbf{N}(u). \quad (29)$$

Note that \mathbf{L} is symmetric, so could be diagonalized.



A single ODE: Exponential integration

The model ODE is

$$u' + cu = F(u). \quad (30)$$

Multiply (30) by the integrating factor e^{ct} :

$$(e^{ct}u)' = e^{ct}F(u).$$

Integrate the above from t_n to $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned} e^{ct_{n+1}}u(t_{n+1}) &= e^{ct_n}u(t_n) + \int_{t_n}^{t_{n+1}} e^{ct}F(u(t)) \, dt \\ &= e^{ct_n}u(t_n) + e^{ct_n} \int_0^{\Delta t} e^{cs}F(u(t_n + s)) \, ds. \end{aligned}$$

Multiply $e^{-ct_{n+1}}$ on both sides:

$$u(t_{n+1}) = e^{-c\Delta t}u(t_n) + e^{-c\Delta t} \int_0^{\Delta t} e^{cs}F(u(t_n + s)) \, ds. \quad (31)$$

First order ETD scheme

$$u(t_{n+1}) = e^{-c\Delta t}u(t_n) + e^{-c\Delta t} \int_0^{\Delta t} e^{cs} \mathbf{F}(u(t_n + s)) \, ds. \quad (31)$$

This formula is exact.

The essence of the ETD methods is *to approximate the integral*.

First order ETD scheme

$$u(t_{n+1}) = e^{-c\Delta t}u(t_n) + e^{-c\Delta t} \int_0^{\Delta t} e^{cs} \mathbf{F}(u(t_n + s)) \, ds. \quad (31)$$

This formula is exact.

The essence of the ETD methods is *to approximate the integral*.

We denote by u_n the approximation to $u(t_n)$ and write $F_n = F(u_n)$.

First order ETD (ETD1) scheme

Using the first order approximation of \mathbf{F} , that is, assuming that F is constant, $F = F_n + \mathcal{O}(\Delta t)$, in $[t_n, t_{n+1}]$, we obtain the ETD1 scheme

$$u_{n+1} = e^{-c\Delta t}u_n + \Delta t \phi_0(c\Delta t)F_n,$$

where $\phi_0(a) = \frac{1-e^{-a}}{a}$.

Remark. In the limit $c \rightarrow 0$,

the ETD1 scheme $\longrightarrow u_{n+1} = u_n + \Delta t F_n$.

Second order ETD multistep scheme

$$u(t_{n+1}) = e^{-c\Delta t}u(t_n) + e^{-c\Delta t} \int_0^{\Delta t} e^{cs} \mathbf{F}(u(t_n + s)) \, ds. \quad (31)$$

Second order ETD multistep (ETDMs2) scheme

Assuming that F is linear, $F = F_n + \frac{F_n - F_{n-1}}{\Delta t}(t - t_n) + \mathcal{O}(\Delta t^2)$, we obtain the ETDMs2 scheme

$$u_{n+1} = e^{-c\Delta t}u_n + \frac{(1 - c\Delta t)e^{-c\Delta t} - 1 + 2c\Delta t}{c^2\Delta t}F_n + \frac{-e^{-c\Delta t} + 1 - c\Delta t}{c^2\Delta t}F_{n-1}.$$

Remark. In the limit $c \rightarrow 0$,

$$\text{the ETDMs2 scheme} \quad \longrightarrow \quad u_{n+1} = u_n + \Delta t \left(\frac{3}{2}F_n - \frac{1}{2}F_{n-1} \right).$$

Second order ETD Runge-Kutta scheme

$$u(t_{n+1}) = e^{-c\Delta t}u(t_n) + e^{-c\Delta t} \int_0^{\Delta t} e^{cs} \mathbf{F}(u(t_n + s)) \, ds. \quad (31)$$

Second order ETD Runge-Kutta (ETDRK2) scheme

First, use the ETD1 scheme to generate

$$\tilde{u}_{n+1} = e^{-c\Delta t}u_n + \frac{1 - e^{-c\Delta t}}{c}F_n.$$

Assuming that F is linear, $F = F_n + \frac{F(\tilde{u}_{n+1}) - F_n}{\Delta t}(t - t_n) + \mathcal{O}(\Delta t^2)$, we obtain the ETDRK2 scheme

$$u_{n+1} = \tilde{u}_{n+1} + \frac{e^{-c\Delta t} - 1 + c\Delta t}{c^2\Delta t}(F(\tilde{u}_{n+1}) - F_n).$$

A system of ODEs: Exponential integration

The model system of ODEs:

$$u_t + Lu = N(u). \quad (29)$$

Pre-multiply (29) by the integrating factor e^{Lt} :

$$(e^{Lt}u)' = e^{Lt}N(u).$$

Integrate the above from t_n to $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned} e^{Lt_{n+1}}u(t_{n+1}) &= e^{Lt_n}u(t_n) + \int_{t_n}^{t_{n+1}} e^{Lt}N(u(t)) \, dt \\ &= e^{Lt_n}u(t_n) + e^{Lt_n} \int_0^{\Delta t} e^{Ls}N(u(t_n + s)) \, ds. \end{aligned}$$

Pre-multiply $e^{-Lt_{n+1}}$ on both sides:

$$u(t_{n+1}) = e^{-L\Delta t}u(t_n) + e^{-L\Delta t} \int_0^{\Delta t} e^{Ls}N(u(t_n + s)) \, ds. \quad (32)$$

First order ETD scheme

$$u(t_{n+1}) = e^{-L\Delta t}u(t_n) + \int_0^{\Delta t} e^{-L(\Delta t-s)} \mathbf{N}(u(t_n + s)) \, ds. \quad (32)$$

The essence of the ETD methods is *to approximate the integral*.

We denote by u_n the approximation of $u(t_n)$.

- approximate $N(u(t_n + s)) \approx N(u(t_n))$ in $s \in [0, \Delta t]$;
- calculate the integral exactly.

ETD1 scheme

$$u_{n+1} = e^{-L\Delta t} u_n + \Delta t \phi_0(L\Delta t) N(u_n),$$

where

$$\phi_0(\mathbf{L}\Delta t) = \int_0^{\Delta t} \mathbf{e}^{-\mathbf{L}(\Delta t-s)} \mathrm{d}s = (\mathbf{L}\Delta t)^{-1}(\mathbf{I} - \mathbf{e}^{-\mathbf{L}\Delta t}).$$

First order ETD scheme (continued)

ETD1 scheme

$$u_{n+1} = e^{-L\Delta t} u_n + \Delta t (L\Delta t)^{-1} (I - e^{-L\Delta t}) N(u_n).$$

Act $e^{L\Delta t}$ on both sides of ETD1:

$$e^{L\Delta t} u_{n+1} = u_n + \Delta t (L\Delta t)^{-1} (e^{L\Delta t} - I) N(u_n).$$

If we approximate $e^{L\Delta t} \approx I + L\Delta t$, then we obtain

$$(I + L\Delta t) u_{n+1} = u_n + \Delta t N(u_n),$$

that is, the first order semi-implicit scheme of (29):

$$\frac{u_{n+1} - u_n}{\Delta t} + L u_{n+1} = N(u_n).$$

Second order ETD multistep scheme

$$u(t_{n+1}) = e^{-L\Delta t}u(t_n) + \int_0^{\Delta t} e^{-L(\Delta t-s)} \mathbf{N}(u(t_n + s)) \, ds. \quad (32)$$

We denote by u_n the approximation of $u(t_n)$.

- approximate

$$\mathbf{N}(u(t_n + s)) \approx \left(1 + \frac{s}{\Delta t}\right) \mathbf{N}(u(t_n)) - \frac{s}{\Delta t} \mathbf{N}(u(t_{n-1})),$$

$$s \in [-\Delta t, \Delta t];$$

- calculate the integral exactly.

ETDMs2 scheme

$$\begin{aligned} u_{n+1} &= e^{-L\Delta t}u_n + \Delta t[(\phi_0 + \phi_1)(L\Delta t)\mathbf{N}(u_n) - \phi_1(L\Delta t)\mathbf{N}(u_{n-1})] \\ &= e^{-L\Delta t}u_n + \Delta t\{\phi_0(L\Delta t)\mathbf{N}(u_n) + \phi_1(L\Delta t)[\mathbf{N}(u_n) - \mathbf{N}(u_{n-1})]\}, \end{aligned}$$

where

$$\phi_1(L\Delta t) = \int_0^{\Delta t} \frac{s}{\Delta t} e^{-L(\Delta t-s)} \, ds = (L\Delta t)^{-2}(L\Delta t - I + e^{-L\Delta t}).$$

Second order ETD Runge-Kutta scheme

$$u(t_{n+1}) = e^{-L\Delta t} u(t_n) + \int_0^{\Delta t} e^{-L(\Delta t-s)} \mathbf{N}(u(t_n + s)) \, ds. \quad (32)$$

We denote by u_n the approximation of $u(t_n)$.

- approximate

$$\mathbf{N}(u(t_n + s)) \approx \left(1 - \frac{s}{\Delta t}\right) \mathbf{N}(u(t_n)) + \frac{s}{\Delta t} \mathbf{N}(u(t_{n+1})), \quad s \in [0, \Delta t],$$

where $u(t_{n+1})$ is approximated by the ETD1 method;

- calculate the integral exactly.

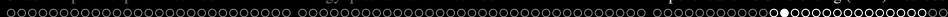
ETDRK2 scheme

$$\tilde{u}_{n+1} = e^{-L\Delta t} u_n + \Delta t \phi_0(L\Delta t) \mathbf{N}(u_n),$$

$$\begin{aligned} u_{n+1} &= e^{-L\Delta t} u_n + \Delta t [(\phi_0 - \phi_1)(L\Delta t) \mathbf{N}(u_n) + \phi_1(L\Delta t) \mathbf{N}(\tilde{u}_{n+1})] \\ &= e^{-L\Delta t} u_n + \Delta t \{ \phi_0(L\Delta t) \mathbf{N}(u_n) + \phi_1(L\Delta t) [\mathbf{N}(\tilde{u}_{n+1}) - \mathbf{N}(u_n)] \}. \end{aligned}$$

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- General theory for ODE systems
- **Example 1. Allen-Cahn equation**
- Example 2. No-slope-selection epitaxial growth model



Allen-Cahn equation

Initial-boundary-value problem of the Allen-Cahn equation:

$$u_t - \varepsilon^2 u_{xx} + u^3 - u = 0, \quad x \in (0, X), \quad t \in (0, T],$$

$$u(\cdot, t) \text{ is } X\text{-periodic}, \quad t \in [0, T],$$

$$u(x, 0) = u_0(x), \quad x \in [0, X].$$

Energy functional:

$$E(u) = \int_{(0,X)} \left(\frac{\varepsilon^2}{2} u_x^2 + \frac{1}{4} (u^2 - 1)^2 \right) dx.$$

We consider

- finite difference method for spatial discretization;
- ETD1 and ETDRK2 methods for temporal integration;
- energy stability for the fully discrete ETD1 scheme.

Spatial discretization: Finite difference method

We use the *central finite difference* to approximate the Laplacian.

- $h = X/N_x$: uniform mesh size;
- $\{x_j = jh : 0 \leq j \leq N_x\}$: nodes on $[0, X]$;
- D_h : the discrete matrix of the Laplacian operator.

Under the periodic boundary conditions, the matrix D_h is given by

$$D_h = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix} \in \mathbb{R}^{N_x \times N_x}.$$

The discrete matrix D_h is symmetric and negative semi-definite.

Spatial discretization: Finite difference method (continued)

The space-discrete scheme: find $v : [0, T] \rightarrow \mathbb{R}^{N_x}$ such that

$$\begin{cases} \frac{dv}{dt} = \varepsilon^2 D_h v + v - v^3, & t \in (0, T], \\ v(0) = v_0. \end{cases}$$

Introduce a stabilizing parameter $S > 0$ and define

$$L_h := -\varepsilon^2 D_h + SI, \quad f(v) := Sv + v - v^3.$$

Then, we obtain

$$\frac{dv}{dt} + L_h v = f(v),$$

whose solution satisfies

$$v(t + \Delta t) = e^{-L_h \Delta t} v(t) + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(v(t+s)) ds.$$

We know L_h is symmetric and positive definite.



ETD methods for the temporal integration

Setting

- $\Delta t = T/N_t$: uniform time step;
- $t_n = n\Delta t$: nodes in the time interval $[0, T]$.

At the time level $t = t_n$, we have

$$v(t_{n+1}) = e^{-L_h \Delta t} v(t_n) + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} \mathbf{f}(v(t_n + s)) \, ds. \quad (33)$$

- approximate $\mathbf{f}(v(t_n + s))$ by $\mathbf{f}(v(t_n))$ in $s \in [0, \Delta t]$,
- calculate the integral exactly.

We obtain the *first order ETD scheme*:

$$\begin{aligned} v^{n+1} &= e^{-L_h \Delta t} v^n + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} \mathbf{f}(v^n) \, ds \\ &= e^{-L_h \Delta t} v^n + \Delta t (L_h \Delta t)^{-1} (I - e^{-L_h \Delta t}) \mathbf{f}(v^n). \end{aligned} \quad (\text{ETD1})$$

ETD methods for the temporal integration (continued)

At the time level $t = t_n$:

$$v(t_{n+1}) = e^{-L_h \Delta t} v(t_n) + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(v(t_n + s)) \, ds. \quad (33)$$

- approximate $f(v(t_n + s))$ by a linear interpolation based on $f(v(t_n))$ and $f(v(t_{n+1}))$,

We obtain the *second order ETD Runge-Kutta scheme*:

$$\begin{cases} \tilde{v}^{n+1} = e^{-L_h \Delta t} v^n + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(v^n) \, ds, \\ v^{n+1} = e^{-L_h \Delta t} v^n + \int_0^{\Delta t} e^{-L_h(\Delta t-s)} \left[\left(1 - \frac{s}{\Delta t}\right) f(v^n) + \frac{s}{\Delta t} f(\tilde{v}^{n+1}) \right] \, ds. \end{cases}$$

(ETDRK2)

Properties of matrix functions

Lemma: Properties of matrix functions

Given a symmetric matrix $M \in \mathbb{R}^{d \times d}$, let ϕ be defined on the spectrum of M , i.e., the values $\{\phi(\lambda_i) : 1 \leq i \leq d\}$ exist, where $\{\lambda_i\}_{i=1}^d$ are the eigenvalues of M . Then

- ① $\phi(M)$ commutes with M ;
- ② $\phi(M^T) = \phi(M)^T$;
- ③ the eigenvalues of $\phi(M)$ are $\phi(\lambda_i)$, $1 \leq i \leq d$;
- ④ $\phi(P^{-1}MP) = P^{-1}\phi(M)P$ for any nonsingular $P \in \mathbb{R}^{d \times d}$.

Example

If $\phi(s) > 0$ for any $s \in \mathbb{R}$, then for any symmetric matrix $M \in \mathbb{R}^{d \times d}$, the matrix $\phi(M)$ is always symmetric and positive definite.

Implementations of matrix exponentials

Letting

$$\phi_{-1}(a) = e^{-a}, \quad \phi_0(a) = \frac{1 - e^{-a}}{a}, \quad \phi_1(a) = \frac{e^{-a} - 1 + a}{a^2},$$

we could write the ETD1 scheme as

$$v^{n+1} = \phi_{-1}(L_h \Delta t) v^n + \Delta t \phi_0(L_h \Delta t) f(v^n),$$

and the ETDRK2 scheme as

$$\begin{cases} \tilde{v}^{n+1} = \phi_{-1}(L_h \Delta t) v^n + \Delta t \phi_0(L_h \Delta t) f(v^n), \\ v^{n+1} = \phi_{-1}(L_h \Delta t) v^n + \Delta t (\phi_0 - \phi_1)(L_h \Delta t) f(v^n) + \Delta t \phi_1(L_h \Delta t) f(\tilde{v}^{n+1}). \end{cases}$$

The actions of exponentials $\phi_\gamma(L_h \Delta t)$ can be implemented efficiently.

Implementations of matrix exponentials (continued)

The exponentials $\phi_\gamma(L_h \Delta t)$ can be implemented by FFT.

Since $L_h = -\varepsilon^2 D_h + SI$ is self-adjoint and positive definite, we have $L_h = P^{-1} \widehat{L}_h P$, where

$$(\widehat{L}_h \hat{f})_k = \lambda_k \hat{f}_k,$$

where $\{\lambda_k\}$ are the eigenvalues of L_h , that is,

$$\lambda_k = \frac{4\varepsilon^2}{h^2} \sin^2 \frac{k\pi}{N_x} + S > 0.$$

Then, we have

$$\phi_\gamma(L_h \Delta t) = P^{-1} \phi_\gamma(\widehat{L}_h \Delta t) P, \quad (\phi_\gamma(\widehat{L}_h \Delta t) \hat{f})_k = \phi_\gamma(\lambda_k \Delta t) \hat{f}_k.$$

P and P^{-1} can be implemented by FFT and iFFT, respectively, so the computational complexity is $\mathcal{O}(N \log N)$ per time step.

Energy stability of the ETD1 scheme

Energy functional:

$$E(u) = \int_{\Omega} F(u) \, dx - \frac{\varepsilon^2}{2} (u, u_{xx}), \quad F(u) = \frac{1}{4} (u^2 - 1)^2.$$

Define the discretized energy E_h :

$$E_h(v) = \sum_{i=1}^{N_x} F(v_i) - \frac{\varepsilon^2}{2} v^T D_h v. \quad (34)$$

Theorem: Energy stability of the ETD1 scheme

Assume that $K := \|F''\|_{L^\infty}$ and $S \geq \frac{K}{2}$. For any $\Delta t > 0$, we have

$$E_h(v^{n+1}) \leq E_h(v^n).$$

Energy stability of the ETD1 scheme (continued)

$$E_h(v) = \sum_{i=1}^{N_x} F(v_i) - \frac{\varepsilon^2}{2} v^T D_h v, \quad f(v) = Sv - F'(v), \quad L_h = S - \varepsilon^2 D_h.$$

Proof. **Step 1.** Direct calculations:

$$E_h(v^{n+1}) - E_h(v^n) = \sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] - \frac{\varepsilon^2}{2} [(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n].$$

We have

$$F(v_i^{n+1}) - F(v_i^n) = F'(v_i^n)(v_i^{n+1} - v_i^n) + \frac{1}{2} F''(\xi)(v_i^{n+1} - v_i^n)^2,$$

then, since $S \geq \frac{1}{2} F''(\xi)$,

$$\begin{aligned} \sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] &\leq (v^{n+1} - v^n)^T F'(v^n) + S(v^{n+1} - v^n)^T (v^{n+1} - v^n) \\ &= S(v^{n+1} - v^n)^T v^{n+1} - (v^{n+1} - v^n)^T f(v^n). \end{aligned}$$

Energy stability of the ETD1 scheme (continued)

$$E_h(v^{n+1}) - E_h(v^n) = \sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] - \frac{\varepsilon^2}{2} [(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n].$$

$$\sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] \leq S(v^{n+1} - v^n)^T v^{n+1} - (v^{n+1} - v^n)^T f(v^n).$$

Direct calculations (using $2a(a - b) = a^2 - b^2 + (a - b)^2$):

$$\begin{aligned} & -\frac{\varepsilon^2}{2} [(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n] \\ &= -\varepsilon^2 (v^{n+1} - v^n)^T D_h v^{n+1} + \frac{\varepsilon^2}{2} (v^{n+1} - v^n)^T D_h (v^{n+1} - v^n) \\ &\leq -\varepsilon^2 (v^{n+1} - v^n)^T D_h v^{n+1} \end{aligned}$$

Then,

$$E_h(v^{n+1}) - E_h(v^n) \leq (v^{n+1} - v^n)^T (L_h v^{n+1} - f(v^n)).$$

Energy stability of the ETD1 scheme (continued)

$$v^{n+1} = e^{-L_h \Delta t} v^n + L_h^{-1} (I - e^{-L_h \Delta t}) f(v^n). \quad (\text{ETD1})$$

$$E_h(v^{n+1}) - E_h(v^n) \leq (v^{n+1} - v^n)^T (L_h v^{n+1} - f(v^n)).$$

Step 2. Solve $f(v^n)$ from (ETD1):

$$\begin{aligned} f(v^n) &= (I - e^{-L_h \Delta t})^{-1} L_h (v^{n+1} - e^{-L_h \Delta t} v^n) \\ &= (I - e^{-L_h \Delta t})^{-1} L_h (v^{n+1} - v^n + (I - e^{-L_h \Delta t}) v^n) \\ &= (I - e^{-L_h \Delta t})^{-1} L_h (v^{n+1} - v^n) + L_h v^n, \end{aligned}$$

and then,

$$\begin{aligned} L_h v^{n+1} - f(v^n) &= L_h (v^{n+1} - v^n) - (I - e^{-L_h \Delta t})^{-1} L_h (v^{n+1} - v^n) \\ &= \Delta t^{-1} B_1 (v^{n+1} - v^n), \end{aligned}$$

where $B_1 := L_h \Delta t - (I - e^{-L_h \Delta t})^{-1} L_h \Delta t$. Then, we obtain

$$E_h(v^{n+1}) - E_h(v^n) \leq \Delta t^{-1} (v^{n+1} - v^n)^T B_1 (v^{n+1} - v^n).$$

Energy stability of the ETD1 scheme (continued)

We have obtained

$$E_h(v^{n+1}) - E_h(v^n) \leq \Delta t^{-1} (v^{n+1} - v^n)^T B_1 (v^{n+1} - v^n),$$

where $B_1 = L_h \Delta t - (I - e^{-L_h \Delta t})^{-1} L_h \Delta t$.

Define a function

$$g_1(a) := a - \frac{a}{1 - e^{-a}}, \quad a \neq 0,$$

then $B_1 = g_1(L_h \Delta t)$. Since

- $g_1(a) < 0$ for any $a > 0$,
- $L_h \Delta t$ is symmetric and positive definite,

we know that B_1 is symmetric and negative definite. So,

$$E_h(v^{n+1}) - E_h(v^n) \leq \Delta t^{-1} (v^{n+1} - v^n)^T B_1 (v^{n+1} - v^n) \leq 0. \quad \square$$

Assume that $K := \|F''\|_{L^\infty}$ and $S \geq \frac{K}{2}$.

- Another topic on the *maximum principle preserving* schemes;
- For some special model, S could be a genetic constant independent on the solution, see the next example.

- Fully implicit schemes
- Convex splitting schemes
- Stabilization schemes

- Invariant energy quadratization (IEQ) schemes
- Scalar auxiliary variable (SAV) schemes

[illegible]

- General theory for ODE systems
- Example 1. Allen-Cahn equation
- **Example 2. No-slope-selection epitaxial growth model**



No-slope-selection epitaxial growth model

Initial-boundary-value problem:

$$u_t + \varepsilon^2 u_{xxxx} + \left(\frac{u_x}{1 + u_x^2} \right)_x = 0, \quad (x, t) \in (0, 2\pi) \times (0, T],$$

$$u(\cdot, t) \text{ is } 2\pi\text{-periodic}, \quad t \in [0, T],$$

$$u(x, 0) = u_0(x), \quad x \in [0, 2\pi].$$

Energy functional:

$$E(u) = \int_{(0, 2\pi)} \left(\frac{\varepsilon^2}{2} u_{xx}^2 - \frac{1}{2} \ln(1 + u_x^2) \right) dx.$$

We consider

- pseudo-spectral method for spatial discretization;
- ETD1 and ETDMs2 methods for temporal integration;
- energy stability for the fully discrete ETD1 scheme.

Linear convex splitting of the energy functional

Consider a splitting of the form $E(u) = E_c(u) - E_e(u)$ as

$$E(u) = \int \left(\frac{A}{2} u_x^2 + \frac{\varepsilon^2}{2} u_{xx}^2 \right) dx - \int \left(\frac{A}{2} u_x^2 + \frac{1}{2} \ln(1 + u_x^2) \right) dx,$$

where $A > 0$ is expected to be as small as possible.

- The convexity of $E_c(u)$ is obvious when $A > 0$.
- The convexity of $E_e(u)$ comes from the convexity of

$$G(a) := \frac{A}{2} a^2 + \frac{1}{2} \ln(1 + a^2), \quad a \in \mathbb{R}.$$

Existence of the linear convex splitting

The function $G(a)$ is convex in \mathbb{R} if and only if $A \geq \frac{1}{8}$.

Linear convex splitting of the energy functional (continued)

Letting $A \geq \frac{1}{8}$ be the stabilizer.

Rewrite the model equation as the splitting form:

$$u_t + \varepsilon^2 u_{xxxx} - Au_{xx} = -\left(\frac{u_x}{1 + u_x^2}\right)_x - Au_{xx}.$$

Due to the periodic boundary condition, we have

$$\int u(x, t) \, dx = \int u_0(x) \, dx, \quad t \in (0, T].$$

Without loss of generality, we assume that the mean of u is zero.

1. *Journal of the American Medical Association*, 1997; 277: 1039-1043.

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1

1. *Journal of Management Studies*, 1996, 33(1), 1-15.

Spatial discretization: Pseudo-spectral method (continued)

For $f \in \mathcal{M}_0$, define the discrete Fourier transform $\hat{f} = Pf$ by

$$\hat{f}_k = \frac{1}{N_x} \sum_{i=1}^{N_x} f_i e^{-ikx_i}, \quad -\frac{N_x}{2} + 1 \leq k \leq \frac{N_x}{2},$$

and f can be reconstructed via $f = P^{-1}\hat{f}$ given by

$$f_i = \sum_{k=-\frac{N_x}{2}+1}^{\frac{N_x}{2}} \hat{f}_k e^{ikx_i}, \quad 1 \leq i \leq N_x.$$

For the discrete version, we can define the operator D_h by

$$D_h v = P^{-1} \hat{D}_h P v, \quad v \in \mathcal{M},$$

where P denotes the discrete Fourier transform, and

$$(\hat{D}_h \hat{v})_k = ik \hat{v}_k, \quad \hat{v} = P v.$$

Spatial discretization: Pseudo-spectral method (continued)

Note that

- $\mathcal{M}_0 = \{f \in \mathcal{M} : \hat{f}_0 = 0\}$.
- $D_h v = 0$ for $v \in \mathcal{M}$ with $v_i = 1$ ($1 \leq i \leq N_x$).

In fact, for (i),

$$\hat{f}_0 = \frac{1}{N_x} \sum_{i=1}^{N_x} f_i.$$

For (ii), we have $\hat{v}_0 = 1$ and for $k \neq 0$,

$$\hat{v}_k = \frac{1}{N_x} \sum_{j=1}^{N_x} (e^{-ijh})^k = \frac{1}{N_x} \cdot \frac{e^{-ijh}(1 - (e^{-ijh})^{N_x})}{1 - e^{-ijh}} = 0.$$

So, $(\hat{D}_h v)_k = 0$ for any k , and then $D_h v = 0$.

Spatial discretization: Pseudo-spectral method (continued)

The space-discrete scheme: find $v : [0, T] \rightarrow \mathbb{R}^{N_x}$ such that

$$\begin{cases} \frac{dv}{dt} + \varepsilon^2 \Delta_h^2 v - A \Delta_h v = -D_h \left(\frac{D_h v}{1 + |D_h v|^2} \right) - A \Delta_h v, & t \in (0, T], \\ v(0) = v_0. \end{cases}$$

Define

$$L_h := \varepsilon^2 \Delta_h^2 - A \Delta_h, \quad f(v) := D_h \left(\frac{D_h v}{1 + |D_h v|^2} \right) + A \Delta_h v.$$

Then, we obtain

$$\frac{dv}{dt} + L_h v = -f(v),$$

whose solution satisfies

$$v(t + \Delta t) = e^{-L_h \Delta t} v(t) - \int_0^{\Delta t} e^{-L_h(\Delta t - s)} f(v(t + s)) ds.$$

We know L_h is symmetric and positive definite since v is mean-zero.

1. *Journal of the American Medical Association*, 2000; 284: 2689-2695.

ETD methods for the temporal integration (continued)

At the time level $t = t_n$, we have

$$v(t_{n+1}) = e^{-L_h \Delta t} v(t_n) - \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(v(t_n + s)) \, ds.$$

- approximating $f(v(t_n + s))$ by $f(v(t_n))$ in $s \in [0, \Delta t]$,
- calculating the integral exactly.

We obtain the *first order ETD scheme*:

$$\begin{aligned} u^{n+1} &= e^{-L_h \Delta t} u^n - \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(u^n) \, ds \\ &= e^{-L_h \Delta t} u^n - L_h^{-1} (I - e^{-L_h \Delta t}) f(u^n). \end{aligned} \tag{ETD1}$$

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

ETD methods for the temporal integration (continued)

ETD1 scheme: $u^{n+1} = e^{-L_h \Delta t} u^n - L_h^{-1} (I - e^{-L_h \Delta t}) f(u^n)$.

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

Proof. We obtain from (ETD1) that

$$\begin{aligned} u^{n+1} - u^n &= -(I - e^{-L_h \Delta t}) u^n - L_h^{-1} (I - e^{-L_h \Delta t}) f(u^n) \\ &= -(I - e^{-L_h \Delta t}) (u^n + L_h^{-1} f(u^n)). \end{aligned}$$

Denote $v \in \mathcal{M}$ with $v_i = 1$ ($1 \leq i \leq N_x$), so $L_h v = 0$. Then,

$$\begin{aligned} \sum_{i=1}^{N_x} (u_i^{n+1} - u_i^n) &= v^T (u^{n+1} - u^n) = -v^T (I - e^{-L_h \Delta t}) (u^n + L_h^{-1} f(u^n)) \\ &= -(u^n + L_h^{-1} f(u^n))^T (I - e^{-L_h \Delta t}) v. \end{aligned}$$

Note that $I - e^{-L_h \Delta t} = L_h \Delta t - \frac{1}{2} (L_h \Delta t)^2 + \dots$, so $(I - e^{-L_h \Delta t}) v = 0$.

ETD methods for the temporal integration (continued)

At the time level $t = t_n$, we have

$$v(t_{n+1}) = e^{-L_h \Delta t} v(t_n) - \int_0^{\Delta t} e^{-L_h(\Delta t-s)} f(v(t_n + s)) \, ds.$$

- approximating $f(v(t_n + s))$ by a linear *extrapolation* based on $f(v(t_n))$ and $f(v(t_{n-1}))$.

We obtain the *second order ETD multistep scheme*:

$$u^{n+1} = e^{-L_h \Delta t} u^n - \int_0^{\Delta t} e^{-L_h(\Delta t-s)} \left[\left(1 + \frac{s}{\Delta t} \right) f(u^n) - \frac{s}{\Delta t} f(u^{n-1}) \right] \, ds.$$

(ETDMs2)

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

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$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(x) e^{-x^2} dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(x) e^{-x^2} dx$$

1. $\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$

Since $L_h = \varepsilon^2 \Delta_h^2 - A \Delta_h$ is self-adjoint and positive definite, we have $L_h = P^{-1} \hat{L}_h P$, where

where $\{\lambda_k\}$ are the eigenvalues of L_h , that is,

Then, we have

P and P^{-1} can be implemented by FFT and iFFT, respectively, so the computational complexity is $\mathcal{O}(N \log N)$ per time step.

Energy stability of the ETD1 scheme

We always assume that $A \geq \frac{1}{8}$.

The discrete energy functional is defined as

$$E_h(u) = \frac{\varepsilon^2}{2} \|\Delta_h u\|_2^2 - \frac{1}{2} \sum_{i=1}^{N_x} \ln(1 + (D_h u)_i^2).$$

ETD1 scheme: $u^{n+1} = e^{-L_h \Delta t} u^n - L_h^{-1}(I - e^{-L_h \Delta t})f(u^n)$.

Theorem: Energy stability of the ETD1 scheme

For any $\Delta t > 0$, we have $E_h(u^{n+1}) \leq E_h(u^n)$.

Basic idea of the proof (similar to Allen-Cahn equation):

- $f(u^n) = -(I - e^{-L_h \Delta t})^{-1} L_h(u^{n+1} - u^n) - L_h u^n$;
- $E_h(u^{n+1}) - E_h(u^n) \leq (u^{n+1} - u^n)^T (L_h u^{n+1} + f(u^n))$
 $= -(u^{n+1} - u^n)^T ((I - e^{-L_h \Delta t})^{-1} - I) L_h (u^{n+1} - u^n)$;
- positive definiteness of $((I - e^{-L_h \Delta t})^{-1} - I) L_h$.

Energy stability of the ETD1 scheme (continued)

$$E_h(u) = \frac{\varepsilon^2}{2} \|\Delta_h u\|_2^2 - \frac{1}{2} \sum_{i=1}^{N_x} \ln(1 + (D_h u)_i^2).$$

Corollary: Uniform H^2 stability of the ETD1 scheme

For any $\Delta t > 0$, we have

$$\max_{1 \leq n \leq N_t} \|\Delta_h u^n\|_2 \leq \frac{2}{\varepsilon} \sqrt{E_h(u^0) + C},$$

where the constant C depends only on ε .

Basic idea of the proof:

- $\ln(1 + y) \leq \alpha y - \ln \alpha + \alpha - 1$ for any $y \geq 0, \alpha \geq 0$;
- discrete Poincaré inequality: $\|D_h u^n\|_2^2 \leq C' \|\Delta_h u^n\|_2^2$;
- $\frac{\varepsilon^2}{4} \|\Delta_h u^n\|_2^2 - C \leq E_h(u^n) \leq E_h(u^{n-1}) \leq \dots \leq E_h(u^0)$.

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